



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 02:37 AM EDT

PDB ID : 2HG4
Title : Structure of the ketosynthase-acyltransferase didomain of module 5 from DEBS.
Authors : Tang, Y.; Kim, C.Y.; Mathews, I.I.; Cane, D.E.; Khosla, C.
Deposited on : 2006-06-26
Resolution : 2.73 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

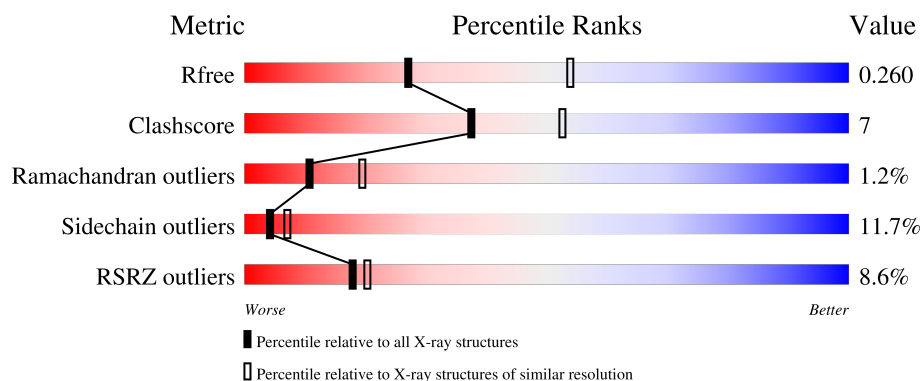
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	917	<div> <div>4%</div> <div>76%</div> <div>16%</div> <div>• •</div> </div>
1	B	917	<div> <div>6%</div> <div>76%</div> <div>17%</div> <div>• •</div> </div>
1	C	917	<div> <div>6%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	D	917	<div> <div>18%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	E	917	<div> <div>8%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	917	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	950	-	-	X	-
2	ACT	C	950	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39402 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 6-Deoxyerythronolide B Synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	B	882	Total	C	N	O	S	Se	0	0	0
			6534	4054	1208	1249	8	15			
1	C	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	D	884	Total	C	N	O	S	Se	0	0	0
			6550	4064	1210	1252	8	16			
1	E	877	Total	C	N	O	S	Se	0	0	0
			6474	4016	1196	1239	8	15			
1	F	874	Total	C	N	O	S	Se	0	0	0
			6440	3995	1189	1233	8	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q5UNP4
A	7	MSE	MET	modified residue	UNP Q5UNP4
A	46	MSE	MET	modified residue	UNP Q5UNP4
A	91	MSE	MET	modified residue	UNP Q5UNP4
A	113	MSE	MET	modified residue	UNP Q5UNP4
A	120	MSE	MET	modified residue	UNP Q5UNP4
A	193	MSE	MET	modified residue	UNP Q5UNP4
A	210	MSE	MET	modified residue	UNP Q5UNP4
A	229	MSE	MET	modified residue	UNP Q5UNP4
A	385	MSE	MET	modified residue	UNP Q5UNP4
A	396	MSE	MET	modified residue	UNP Q5UNP4
A	480	MSE	MET	modified residue	UNP Q5UNP4
A	525	GLU	ASP	conflict	UNP Q5UNP4
A	555	MSE	MET	modified residue	UNP Q5UNP4
A	567	MSE	MET	modified residue	UNP Q5UNP4
A	621	MSE	MET	modified residue	UNP Q5UNP4
A	680	MSE	MET	modified residue	UNP Q5UNP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	732	ALA	GLY	conflict	UNP Q5UNP4
A	733	HIS	ILE	conflict	UNP Q5UNP4
A	734	LYS	THR	conflict	UNP Q5UNP4
A	786	MSE	MET	modified residue	UNP Q5UNP4
B	1	MSE	MET	modified residue	UNP Q5UNP4
B	7	MSE	MET	modified residue	UNP Q5UNP4
B	46	MSE	MET	modified residue	UNP Q5UNP4
B	91	MSE	MET	modified residue	UNP Q5UNP4
B	113	MSE	MET	modified residue	UNP Q5UNP4
B	120	MSE	MET	modified residue	UNP Q5UNP4
B	193	MSE	MET	modified residue	UNP Q5UNP4
B	210	MSE	MET	modified residue	UNP Q5UNP4
B	229	MSE	MET	modified residue	UNP Q5UNP4
B	385	MSE	MET	modified residue	UNP Q5UNP4
B	396	MSE	MET	modified residue	UNP Q5UNP4
B	480	MSE	MET	modified residue	UNP Q5UNP4
B	525	GLU	ASP	conflict	UNP Q5UNP4
B	555	MSE	MET	modified residue	UNP Q5UNP4
B	567	MSE	MET	modified residue	UNP Q5UNP4
B	621	MSE	MET	modified residue	UNP Q5UNP4
B	680	MSE	MET	modified residue	UNP Q5UNP4
B	732	ALA	GLY	conflict	UNP Q5UNP4
B	733	HIS	ILE	conflict	UNP Q5UNP4
B	734	LYS	THR	conflict	UNP Q5UNP4
B	786	MSE	MET	modified residue	UNP Q5UNP4
C	1	MSE	MET	modified residue	UNP Q5UNP4
C	7	MSE	MET	modified residue	UNP Q5UNP4
C	46	MSE	MET	modified residue	UNP Q5UNP4
C	91	MSE	MET	modified residue	UNP Q5UNP4
C	113	MSE	MET	modified residue	UNP Q5UNP4
C	120	MSE	MET	modified residue	UNP Q5UNP4
C	193	MSE	MET	modified residue	UNP Q5UNP4
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C	385	MSE	MET	modified residue	UNP Q5UNP4
C	396	MSE	MET	modified residue	UNP Q5UNP4
C	480	MSE	MET	modified residue	UNP Q5UNP4
C	525	GLU	ASP	conflict	UNP Q5UNP4
C	555	MSE	MET	modified residue	UNP Q5UNP4
C	567	MSE	MET	modified residue	UNP Q5UNP4
C	621	MSE	MET	modified residue	UNP Q5UNP4
C	680	MSE	MET	modified residue	UNP Q5UNP4

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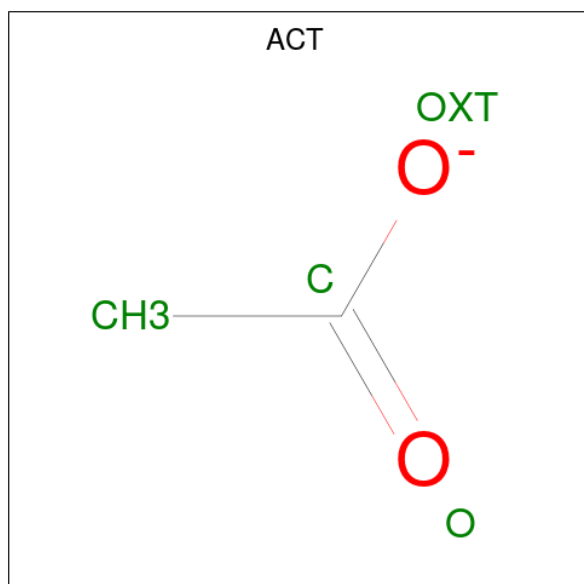
Chain	Residue	Modelled	Actual	Comment	Reference
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C	733	HIS	ILE	conflict	UNP Q5UNP4
C	734	LYS	THR	conflict	UNP Q5UNP4
C	786	MSE	MET	modified residue	UNP Q5UNP4
D	1	MSE	MET	modified residue	UNP Q5UNP4
D	7	MSE	MET	modified residue	UNP Q5UNP4
D	46	MSE	MET	modified residue	UNP Q5UNP4
D	91	MSE	MET	modified residue	UNP Q5UNP4
D	113	MSE	MET	modified residue	UNP Q5UNP4
D	120	MSE	MET	modified residue	UNP Q5UNP4
D	193	MSE	MET	modified residue	UNP Q5UNP4
D	210	MSE	MET	modified residue	UNP Q5UNP4
D	229	MSE	MET	modified residue	UNP Q5UNP4
D	385	MSE	MET	modified residue	UNP Q5UNP4
D	396	MSE	MET	modified residue	UNP Q5UNP4
D	480	MSE	MET	modified residue	UNP Q5UNP4
D	525	GLU	ASP	conflict	UNP Q5UNP4
D	555	MSE	MET	modified residue	UNP Q5UNP4
D	567	MSE	MET	modified residue	UNP Q5UNP4
D	621	MSE	MET	modified residue	UNP Q5UNP4
D	680	MSE	MET	modified residue	UNP Q5UNP4
D	732	ALA	GLY	conflict	UNP Q5UNP4
D	733	HIS	ILE	conflict	UNP Q5UNP4
D	734	LYS	THR	conflict	UNP Q5UNP4
D	786	MSE	MET	modified residue	UNP Q5UNP4
E	1	MSE	MET	modified residue	UNP Q5UNP4
E	7	MSE	MET	modified residue	UNP Q5UNP4
E	46	MSE	MET	modified residue	UNP Q5UNP4
E	91	MSE	MET	modified residue	UNP Q5UNP4
E	113	MSE	MET	modified residue	UNP Q5UNP4
E	120	MSE	MET	modified residue	UNP Q5UNP4
E	193	MSE	MET	modified residue	UNP Q5UNP4
E	210	MSE	MET	modified residue	UNP Q5UNP4
E	229	MSE	MET	modified residue	UNP Q5UNP4
E	385	MSE	MET	modified residue	UNP Q5UNP4
E	396	MSE	MET	modified residue	UNP Q5UNP4
E	480	MSE	MET	modified residue	UNP Q5UNP4
E	525	GLU	ASP	conflict	UNP Q5UNP4
E	555	MSE	MET	modified residue	UNP Q5UNP4
E	567	MSE	MET	modified residue	UNP Q5UNP4
E	621	MSE	MET	modified residue	UNP Q5UNP4
E	680	MSE	MET	modified residue	UNP Q5UNP4

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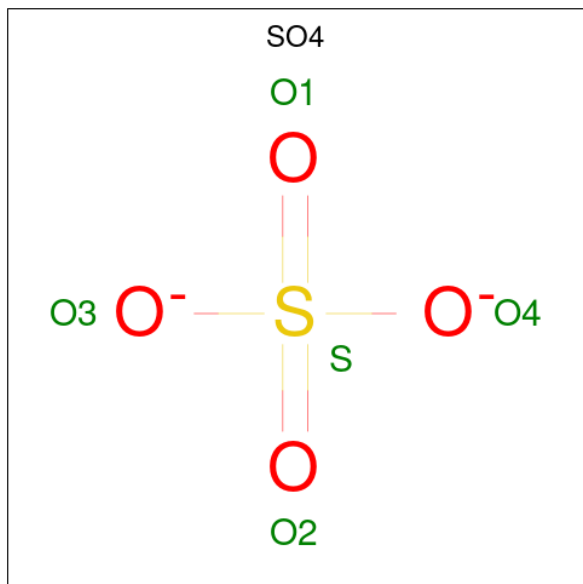
Chain	Residue	Modelled	Actual	Comment	Reference
E	732	ALA	GLY	conflict	UNP Q5UNP4
E	733	HIS	ILE	conflict	UNP Q5UNP4
E	734	LYS	THR	conflict	UNP Q5UNP4
E	786	MSE	MET	modified residue	UNP Q5UNP4
F	1	MSE	MET	modified residue	UNP Q5UNP4
F	7	MSE	MET	modified residue	UNP Q5UNP4
F	46	MSE	MET	modified residue	UNP Q5UNP4
F	91	MSE	MET	modified residue	UNP Q5UNP4
F	113	MSE	MET	modified residue	UNP Q5UNP4
F	120	MSE	MET	modified residue	UNP Q5UNP4
F	193	MSE	MET	modified residue	UNP Q5UNP4
F	210	MSE	MET	modified residue	UNP Q5UNP4
F	229	MSE	MET	modified residue	UNP Q5UNP4
F	385	MSE	MET	modified residue	UNP Q5UNP4
F	396	MSE	MET	modified residue	UNP Q5UNP4
F	480	MSE	MET	modified residue	UNP Q5UNP4
F	525	GLU	ASP	conflict	UNP Q5UNP4
F	555	MSE	MET	modified residue	UNP Q5UNP4
F	567	MSE	MET	modified residue	UNP Q5UNP4
F	621	MSE	MET	modified residue	UNP Q5UNP4
F	680	MSE	MET	modified residue	UNP Q5UNP4
F	732	ALA	GLY	conflict	UNP Q5UNP4
F	733	HIS	ILE	conflict	UNP Q5UNP4
F	734	LYS	THR	conflict	UNP Q5UNP4
F	786	MSE	MET	modified residue	UNP Q5UNP4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0

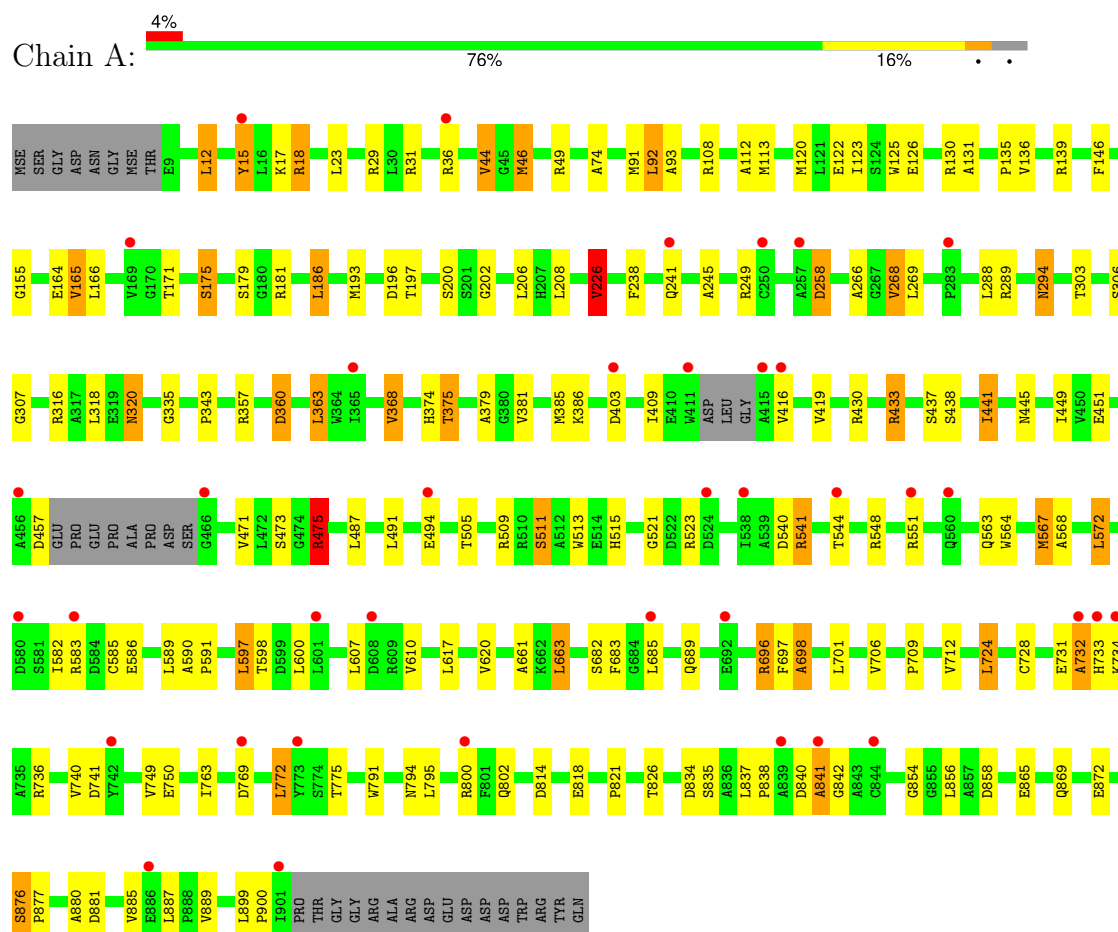
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total 74	O 74	0	0
5	B	57	Total 57	O 57	0	0
5	C	42	Total 42	O 42	0	0
5	D	50	Total 50	O 50	0	0
5	E	49	Total 49	O 49	0	0
5	F	38	Total 38	O 38	0	0

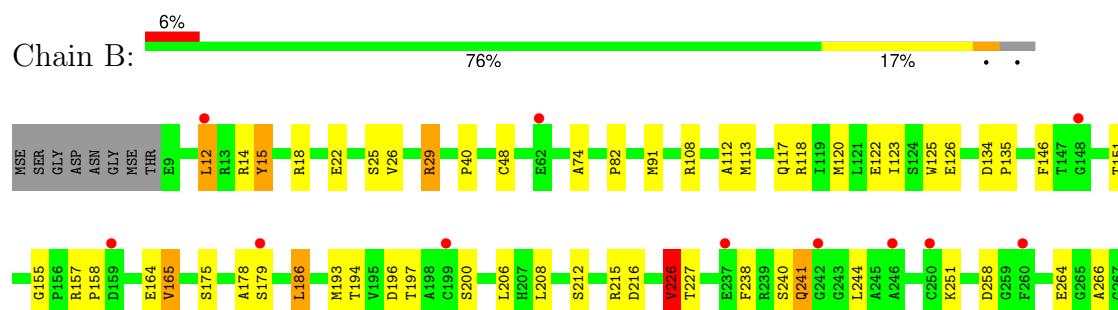
3 Residue-property plots

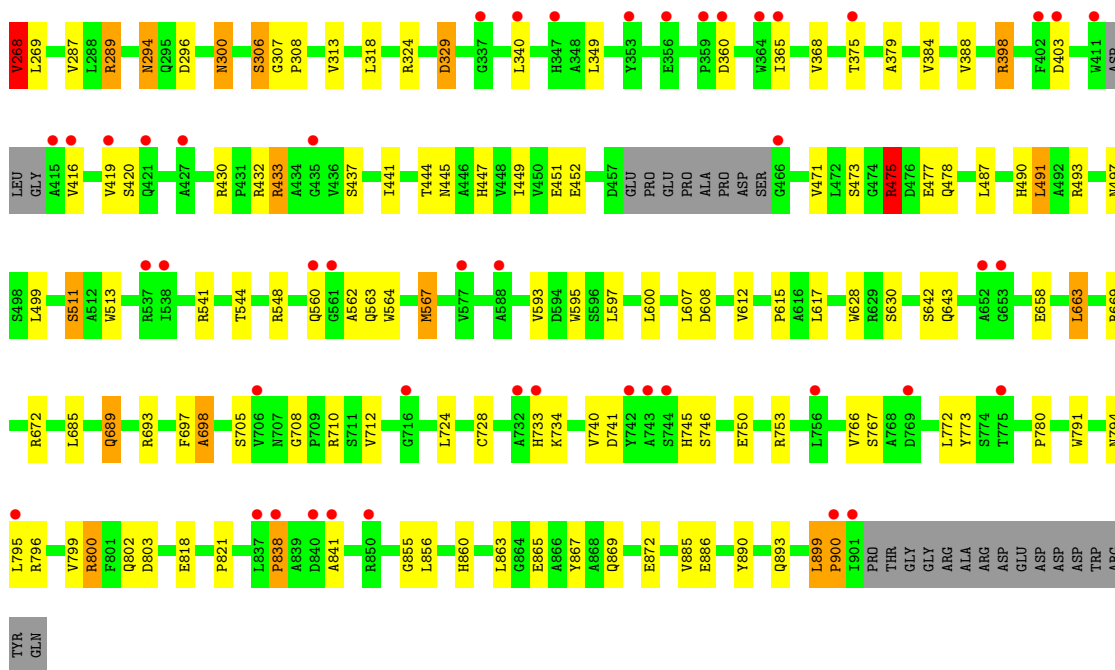
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 6-Deoxyerythronolide B Synthase

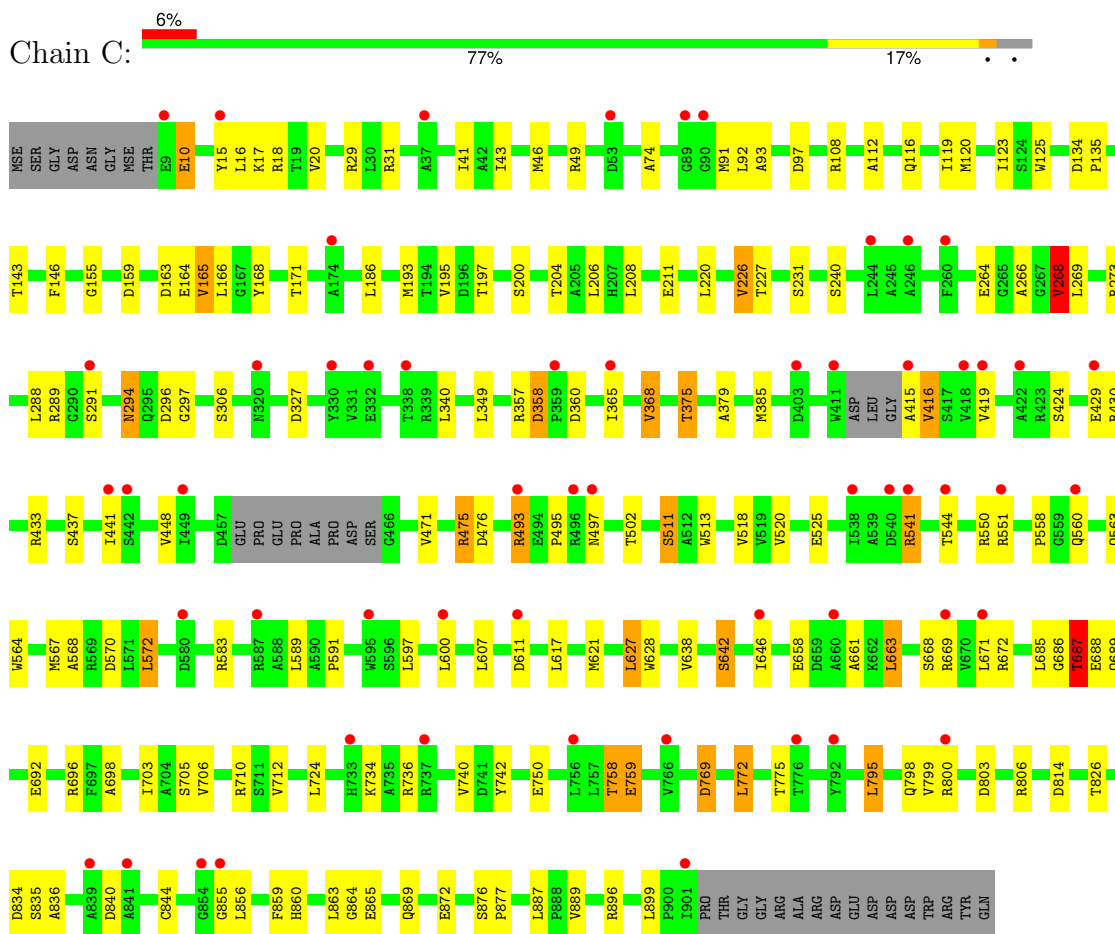


• Molecule 1: 6-Deoxyerythronolide B Synthase

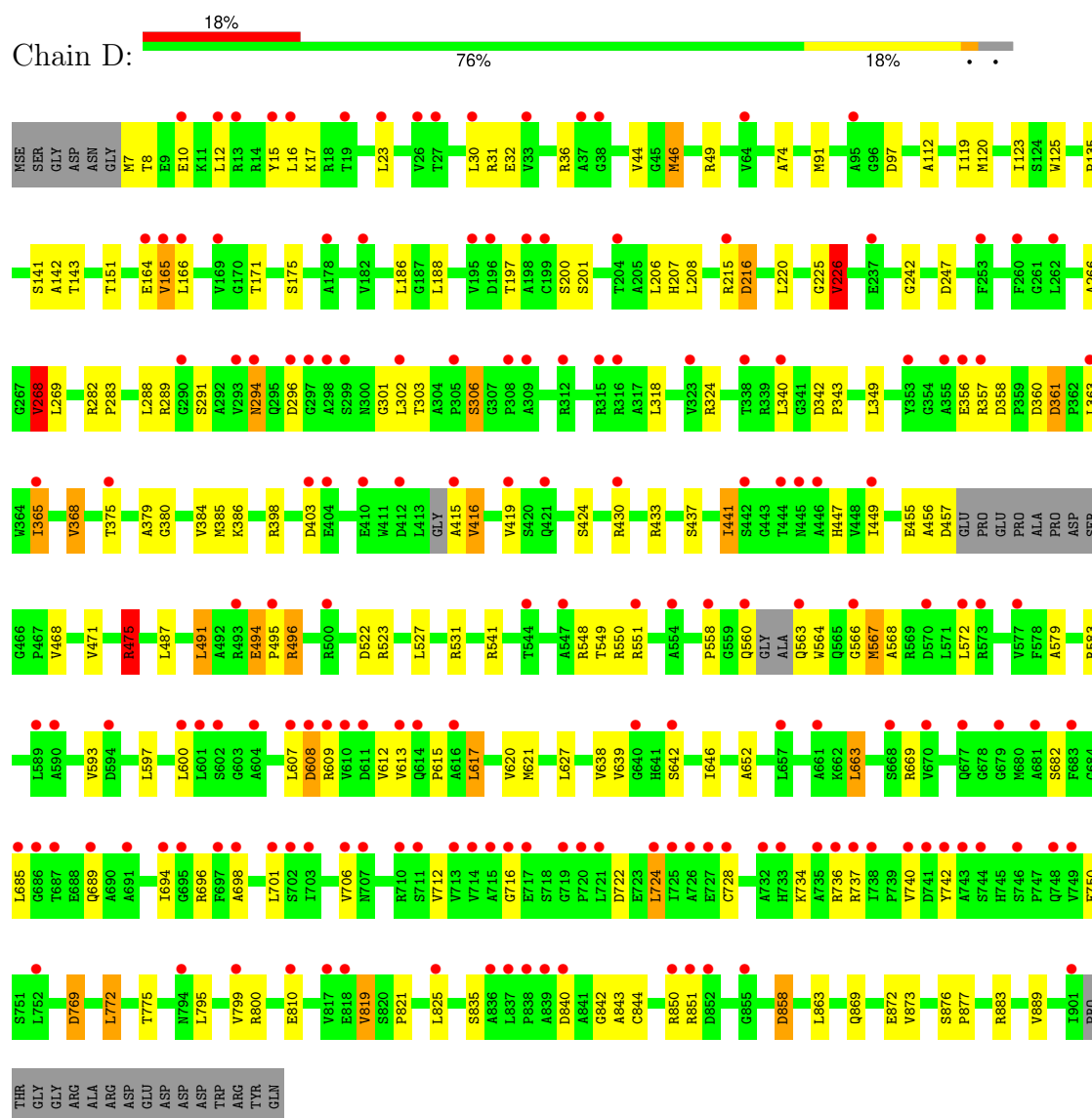




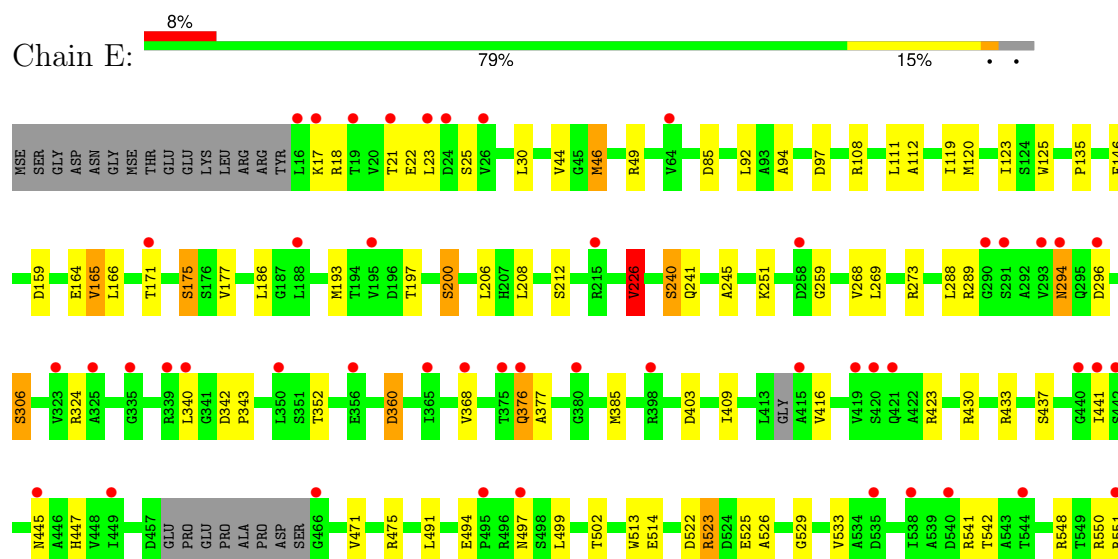
- Molecule 1: 6-Deoxyerythronolide B Synthase

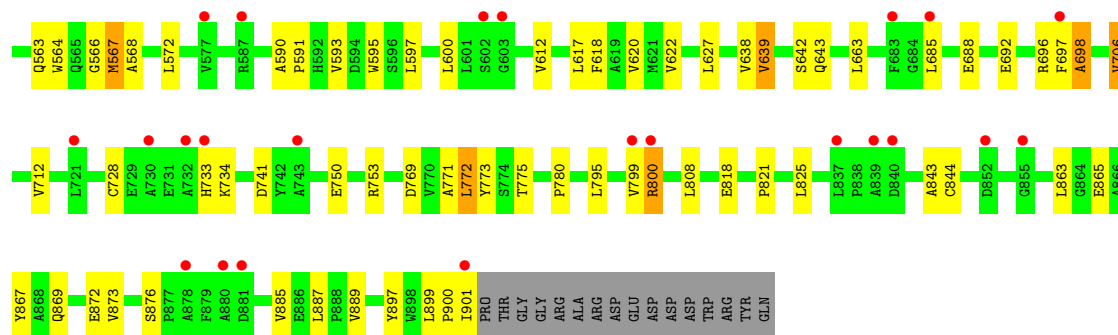


- Molecule 1: 6-Deoxyerythronolide B Synthase

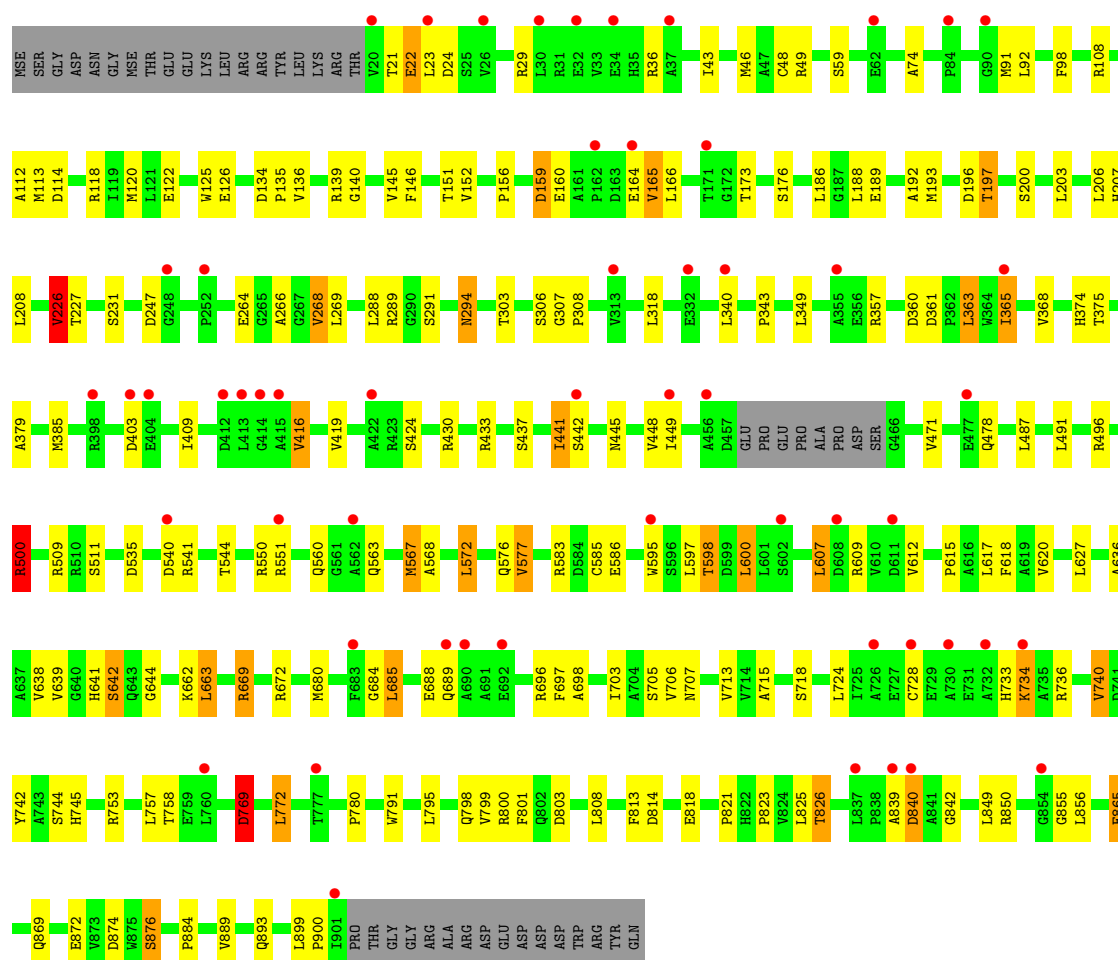
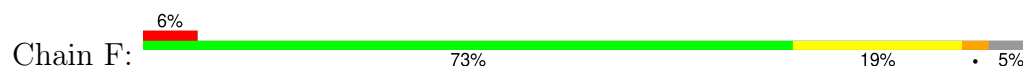


- Molecule 1: 6-Deoxyerythronolide B Synthase





• Molecule 1: 6-Deoxyerythronolide B Synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	305.26Å 150.15Å 184.38Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	48.03 – 2.73 48.03 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.73) 99.8 (48.03-2.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.255 0.223 , 0.260	Depositor DCC
R_{free} test set	10395 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	39402	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.71	1/6634 (0.0%)	0.79	7/8999 (0.1%)
1	B	0.63	1/6648 (0.0%)	0.76	5/9015 (0.1%)
1	C	0.64	1/6634 (0.0%)	0.74	2/8999 (0.0%)
1	D	0.60	0/6663	0.73	5/9034 (0.1%)
1	E	0.58	0/6587	0.71	1/8936 (0.0%)
1	F	0.66	2/6554 (0.0%)	0.77	5/8894 (0.1%)
All	All	0.64	5/39720 (0.0%)	0.75	25/53877 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	3
1	F	0	2
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	872	GLU	CG-CD	7.16	1.62	1.51
1	B	48	CYS	CB-SG	-5.58	1.72	1.81
1	C	211	GLU	CG-CD	5.11	1.59	1.51
1	F	585	CYS	CB-SG	-5.11	1.73	1.81
1	A	585	CYS	CB-SG	-5.10	1.73	1.81

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	D	475	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	F	226	VAL	CB-CA-C	-7.03	98.05	111.40
1	A	226	VAL	CB-CA-C	-6.84	98.40	111.40
1	A	475	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	226	VAL	CB-CA-C	-6.38	99.27	111.40
1	B	475	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	E	226	VAL	CB-CA-C	-6.22	99.59	111.40
1	F	500	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	475	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	130	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	226	VAL	CB-CA-C	-5.59	100.77	111.40
1	C	368	VAL	CB-CA-C	-5.59	100.78	111.40
1	D	368	VAL	CB-CA-C	-5.53	100.90	111.40
1	F	268	VAL	CB-CA-C	-5.43	101.08	111.40
1	A	15	TYR	CA-CB-CG	-5.38	103.18	113.40
1	B	268	VAL	CB-CA-C	-5.37	101.20	111.40
1	C	268	VAL	CB-CA-C	-5.37	101.20	111.40
1	D	268	VAL	CB-CA-C	-5.35	101.23	111.40
1	F	36	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	475	ARG	CG-CD-NE	5.23	122.79	111.80
1	A	363	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	493	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	475	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	F	842	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLY	Peptide
1	A	840	ASP	Peptide
1	A	841	ALA	Peptide
1	A	842	GLY	Peptide
1	B	155	GLY	Peptide
1	C	10	GLU	Peptide
1	C	155	GLY	Peptide
1	C	840	ASP	Peptide
1	F	21	THR	Peptide
1	F	22	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6520	0	6359	84	0
1	B	6534	0	6385	100	0
1	C	6520	0	6359	97	0
1	D	6550	0	6396	91	0
1	E	6474	0	6316	75	0
1	F	6440	0	6274	97	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
2	C	4	0	3	4	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	74	0	0	3	0
5	B	57	0	0	1	0
5	C	42	0	0	5	0
5	D	50	0	0	1	0
5	E	49	0	0	3	0
5	F	38	0	0	1	0
All	All	39402	0	38107	533	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (533) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:SER:OG	2:B:950:ACT:O	1.71	1.06
1:F:207:HIS:HD1	1:F:291:SER:HG	1.16	0.94
1:D:617:LEU:HD22	1:D:621:MSE:HE3	1.53	0.91
1:C:193:MSE:HE3	1:C:208:LEU:HD13	1.56	0.86
1:E:564:TRP:O	1:E:567:MSE:HG3	1.78	0.84
1:A:865:GLU:O	1:A:869:GLN:HG3	1.78	0.83
1:A:193:MSE:HE3	1:A:208:LEU:HD13	1.60	0.83
1:D:294:ASN:C	1:D:294:ASN:HD22	1.81	0.81
1:D:349:LEU:HD13	1:D:365:ILE:HD11	1.62	0.80
1:F:586:GLU:OE1	1:F:598:THR:OG1	2.01	0.79
1:A:294:ASN:C	1:A:294:ASN:HD22	1.86	0.79
1:B:193:MSE:HE3	1:B:208:LEU:HD13	1.65	0.77
1:A:245:ALA:HA	1:A:258:ASP:HB2	1.64	0.77
1:F:193:MSE:HE3	1:F:208:LEU:HD13	1.69	0.74
1:F:294:ASN:C	1:F:294:ASN:HD22	1.92	0.73
1:D:701:LEU:HD23	1:D:716:GLY:HA3	1.70	0.72
1:C:294:ASN:C	1:C:294:ASN:HD22	1.94	0.72
1:D:620:VAL:HG11	1:D:821:PRO:HG3	1.71	0.72
1:A:193:MSE:CE	1:A:208:LEU:HD13	2.18	0.71
1:D:120:MSE:HE3	1:D:226:VAL:HG22	1.72	0.71
1:C:46:MSE:HB2	1:C:385:MSE:HE2	1.71	0.71
1:B:120:MSE:HE3	1:B:226:VAL:HG13	1.72	0.71
1:C:120:MSE:HE3	1:C:226:VAL:HG13	1.71	0.71
1:B:564:TRP:O	1:B:567:MSE:HG3	1.90	0.70
1:C:493:ARG:O	1:C:495:PRO:HD3	1.90	0.70
1:B:120:MSE:CE	1:B:123:ILE:HD11	2.22	0.69
1:A:136:VAL:O	1:A:139:ARG:HG3	1.92	0.69
1:C:558:PRO:HD2	1:C:621:MSE:SE	2.42	0.69
1:C:688:GLU:O	1:C:692:GLU:HG2	1.93	0.69
1:D:296:ASP:HB2	1:D:306:SER:HB3	1.75	0.69
1:D:617:LEU:CD2	1:D:621:MSE:HE3	2.23	0.69
1:A:320:ASN:N	1:A:320:ASN:HD22	1.88	0.69
1:B:294:ASN:C	1:B:294:ASN:HD22	1.95	0.69
1:B:197:THR:HG22	1:B:197:THR:O	1.93	0.68
1:B:251:LYS:NZ	1:B:258:ASP:OD2	2.28	0.67
1:E:17:LYS:O	1:E:21:THR:OG1	2.08	0.67
1:E:294:ASN:HD22	1:E:294:ASN:C	1.98	0.67
1:B:241:GLN:HE21	1:B:241:GLN:C	1.98	0.66
1:B:437:SER:HB3	1:B:447:HIS:ND1	2.11	0.66
1:E:642:SER:OG	2:E:950:ACT:C	2.43	0.66
1:A:197:THR:HG22	1:A:197:THR:O	1.94	0.65
1:A:15:TYR:CE1	1:A:18:ARG:HD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:HB2	1:B:165:VAL:HG22	1.79	0.65
1:B:193:MSE:CE	1:B:208:LEU:HD13	2.27	0.65
1:F:705:SER:CB	1:F:799:VAL:HB	2.27	0.65
1:A:206:LEU:HD21	1:A:288:LEU:HD13	1.78	0.64
1:B:146:PHE:HD1	1:B:193:MSE:HE2	1.62	0.64
1:F:206:LEU:HD21	1:F:288:LEU:HD13	1.79	0.64
1:F:728:CYS:HB3	1:F:733:HIS:HB2	1.78	0.64
1:A:112:ALA:HB2	1:A:165:VAL:HG22	1.80	0.64
1:D:724:LEU:O	1:D:728:CYS:SG	2.48	0.64
1:A:120:MSE:HE3	1:A:226:VAL:HG13	1.79	0.63
1:D:361:ASP:OD1	1:D:361:ASP:O	2.16	0.63
1:D:120:MSE:HE1	1:D:266:ALA:HB1	1.80	0.63
1:E:112:ALA:HB2	1:E:165:VAL:HG22	1.81	0.63
1:E:494:GLU:HB3	1:E:497:ASN:HD22	1.63	0.62
1:F:43:ILE:HG21	1:F:46:MSE:HE3	1.81	0.62
1:F:136:VAL:O	1:F:139:ARG:HG3	1.99	0.62
1:B:146:PHE:CD1	1:B:193:MSE:HE2	2.34	0.62
1:E:120:MSE:CE	1:E:123:ILE:HD11	2.30	0.62
1:D:475:ARG:HH11	1:D:475:ARG:HG3	1.65	0.62
1:F:206:LEU:C	1:F:206:LEU:HD23	2.20	0.61
1:B:296:ASP:HB2	1:B:306:SER:HB3	1.82	0.61
1:E:706:VAL:HG22	1:E:800:ARG:HA	1.83	0.61
1:E:566:GLY:O	1:E:568:ALA:N	2.34	0.61
1:C:206:LEU:HD21	1:C:288:LEU:HD13	1.83	0.61
1:D:638:VAL:HG23	1:D:772:LEU:HD22	1.84	0.60
1:C:43:ILE:HG21	1:C:46:MSE:HE3	1.82	0.60
1:C:193:MSE:CE	1:C:208:LEU:HD13	2.29	0.60
1:D:294:ASN:C	1:D:294:ASN:ND2	2.52	0.60
1:D:609:ARG:O	1:D:613:VAL:HG23	2.01	0.60
1:E:146:PHE:HD2	1:E:193:MSE:HE2	1.66	0.60
1:D:197:THR:HG22	1:D:197:THR:O	2.02	0.60
1:E:197:THR:O	1:E:197:THR:HG22	2.02	0.60
1:D:120:MSE:SE	1:D:226:VAL:HG22	2.52	0.60
1:F:595:TRP:CZ2	1:F:612:VAL:HA	2.35	0.60
1:F:638:VAL:HG23	1:F:772:LEU:HD22	1.84	0.60
1:A:268:VAL:O	1:A:269:LEU:HD12	2.02	0.60
1:C:296:ASP:HB2	1:C:306:SER:HB3	1.82	0.60
1:E:638:VAL:HG23	1:E:772:LEU:HD22	1.84	0.59
1:F:120:MSE:HE3	1:F:226:VAL:HG13	1.82	0.59
1:F:197:THR:CG2	1:F:197:THR:O	2.51	0.58
1:E:437:SER:HB3	1:E:447:HIS:ND1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ILE:HD12	1:E:268:VAL:HG23	1.86	0.58
1:E:197:THR:HG22	1:E:200:SER:OG	2.02	0.58
1:D:120:MSE:HE3	1:D:226:VAL:HG13	1.85	0.58
1:F:146:PHE:HD2	1:F:193:MSE:HE2	1.68	0.58
1:A:294:ASN:C	1:A:294:ASN:ND2	2.56	0.58
1:A:564:TRP:O	1:A:567:MSE:HG3	2.03	0.58
1:C:560:GLN:NE2	1:C:742:TYR:OH	2.36	0.58
1:E:595:TRP:CZ2	1:E:612:VAL:HA	2.39	0.58
1:A:854:GLY:O	1:A:858:ASP:OD2	2.21	0.58
1:C:206:LEU:HD23	1:C:206:LEU:O	2.04	0.57
1:F:193:MSE:CE	1:F:208:LEU:HD13	2.34	0.57
1:F:471:VAL:HG12	5:F:992:HOH:O	2.03	0.57
1:B:289:ARG:HH11	1:B:289:ARG:HG2	1.69	0.57
1:C:865:GLU:O	1:C:869:GLN:HG3	2.03	0.57
1:D:120:MSE:CE	1:D:226:VAL:HG22	2.34	0.57
1:F:707:ASN:HD21	1:F:713:VAL:HG23	1.68	0.57
1:E:22:GLU:HB3	1:F:23:LEU:HD21	1.86	0.57
1:C:591:PRO:HD3	1:F:478:GLN:HE22	1.70	0.57
1:C:642:SER:OG	2:C:950:ACT:C	2.53	0.57
1:D:722:ASP:OD1	1:D:737:ARG:NH2	2.38	0.57
1:C:564:TRP:O	1:C:567:MSE:HG3	2.05	0.56
1:F:227:THR:O	1:F:264:GLU:HB2	2.04	0.56
1:F:294:ASN:ND2	1:F:445:ASN:HB2	2.19	0.56
1:B:120:MSE:HE1	1:B:123:ILE:HD11	1.86	0.56
1:D:46:MSE:CE	1:D:385:MSE:HG2	2.35	0.56
1:F:156:PRO:HB2	1:F:160:GLU:HG3	1.87	0.56
1:F:197:THR:O	1:F:197:THR:HG22	2.05	0.56
1:F:620:VAL:HG11	1:F:821:PRO:HG3	1.88	0.56
1:B:108:ARG:HD3	1:B:164:GLU:O	2.05	0.56
1:B:475:ARG:HG3	1:B:475:ARG:HH11	1.70	0.56
1:B:375:THR:HG23	1:B:379:ALA:N	2.21	0.56
1:C:799:VAL:HG22	5:C:1018:HOH:O	2.06	0.56
1:D:437:SER:HB3	1:D:447:HIS:ND1	2.20	0.56
1:B:595:TRP:CZ2	1:B:612:VAL:HA	2.41	0.56
1:C:120:MSE:HE1	1:C:123:ILE:HD11	1.88	0.56
1:B:773:TYR:HA	1:B:780:PRO:HA	1.88	0.55
1:B:289:ARG:HG2	1:B:289:ARG:NH1	2.19	0.55
1:C:197:THR:HG22	1:C:197:THR:O	2.06	0.55
1:D:32:GLU:OE1	1:D:36:ARG:CZ	2.54	0.55
1:D:197:THR:HG22	1:D:200:SER:OG	2.06	0.55
1:E:901:ILE:C	5:E:1002:HOH:O	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MSE:HE1	1:D:15:TYR:CE2	2.42	0.55
1:F:146:PHE:CD2	1:F:193:MSE:HE2	2.42	0.55
1:B:113:MSE:HE2	1:B:118:ARG:HG2	1.89	0.55
1:F:705:SER:HB2	1:F:799:VAL:HB	1.88	0.55
1:B:766:VAL:HG12	1:B:767:SER:O	2.06	0.55
1:D:375:THR:HG23	1:D:379:ALA:N	2.22	0.54
1:B:499:LEU:N	3:B:975:SO4:O1	2.31	0.54
1:E:146:PHE:CD2	1:E:193:MSE:HE2	2.43	0.54
1:B:12:LEU:HD12	1:B:15:TYR:HD2	1.72	0.54
1:F:120:MSE:HE1	1:F:266:ALA:HB1	1.89	0.54
1:C:108:ARG:HD2	1:C:168:TYR:HE2	1.70	0.54
1:D:215:ARG:O	1:D:216:ASP:HB2	2.07	0.54
1:E:728:CYS:HB3	1:E:733:HIS:HB2	1.89	0.54
1:C:876:SER:HB2	1:C:877:PRO:HD3	1.90	0.54
1:D:858:ASP:N	1:D:858:ASP:OD1	2.40	0.54
1:E:523:ARG:O	1:E:526:ALA:HB3	2.08	0.54
1:C:15:TYR:HE2	1:E:551:ARG:CZ	2.21	0.54
1:D:769:ASP:OD1	1:D:769:ASP:N	2.30	0.53
1:B:728:CYS:HB3	1:B:733:HIS:HB2	1.90	0.53
1:A:74:ALA:HA	1:A:91:MSE:HG3	1.91	0.53
1:F:821:PRO:HA	1:F:849:LEU:HB2	1.90	0.53
1:C:195:VAL:HG21	1:C:208:LEU:HD12	1.90	0.53
1:C:227:THR:O	1:C:264:GLU:HB2	2.09	0.53
1:F:294:ASN:C	1:F:294:ASN:ND2	2.59	0.53
1:D:455:GLU:OE1	1:D:455:GLU:HA	2.08	0.53
1:A:197:THR:O	1:A:197:THR:CG2	2.56	0.53
1:C:15:TYR:CE2	1:E:551:ARG:CZ	2.93	0.52
1:D:775:THR:O	1:D:799:VAL:O	2.27	0.52
1:C:710:ARG:CG	1:C:710:ARG:O	2.56	0.52
1:D:527:LEU:O	1:D:531:ARG:HG3	2.09	0.52
1:F:349:LEU:HD13	1:F:365:ILE:HD11	1.90	0.52
1:B:433:ARG:NH1	1:B:451:GLU:OE1	2.42	0.52
1:C:475:ARG:HD3	1:C:513:TRP:CD2	2.44	0.52
1:B:25:SER:O	1:B:29:ARG:HB2	2.09	0.52
1:B:113:MSE:HE2	1:B:118:ARG:CG	2.40	0.52
1:C:415:ALA:HB1	5:C:1006:HOH:O	2.08	0.52
1:E:620:VAL:HG11	1:E:821:PRO:HG3	1.92	0.52
1:A:343:PRO:HA	1:A:409:ILE:HG12	1.91	0.52
1:C:358:ASP:N	1:C:358:ASP:OD1	2.43	0.52
1:B:669:ARG:HG2	1:B:672:ARG:HH12	1.75	0.52
1:A:433:ARG:NH1	1:A:451:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:O	1:B:216:ASP:HB2	2.09	0.52
1:F:874:ASP:OD1	1:F:876:SER:OG	2.19	0.52
1:A:294:ASN:ND2	1:A:445:ASN:HB2	2.26	0.51
1:A:505:THR:HB	1:A:887:LEU:HD11	1.92	0.51
1:C:646:ILE:HG12	1:C:663:LEU:HD13	1.91	0.51
1:D:120:MSE:CE	1:D:266:ALA:HB1	2.40	0.51
1:F:576:GLN:O	1:F:577:VAL:C	2.49	0.51
1:E:865:GLU:O	1:E:869:GLN:HG3	2.10	0.51
1:F:639:VAL:CG2	1:F:808:LEU:HD11	2.40	0.51
1:D:642:SER:OG	2:D:950:ACT:C	2.59	0.51
1:C:268:VAL:C	1:C:269:LEU:HD12	2.31	0.51
1:E:108:ARG:HD3	1:E:164:GLU:O	2.11	0.51
1:A:521:GLY:HA2	5:A:1000:HOH:O	2.10	0.51
1:C:710:ARG:O	1:C:710:ARG:HG2	2.11	0.51
1:D:560:GLN:NE2	1:D:742:TYR:OH	2.40	0.51
1:B:123:ILE:HD12	1:B:268:VAL:CG2	2.41	0.51
1:C:638:VAL:HG23	1:C:772:LEU:HD22	1.92	0.51
1:E:818:GLU:OE2	1:E:825:LEU:N	2.39	0.51
1:C:116:GLN:O	1:C:120:MSE:HG2	2.11	0.51
1:E:22:GLU:HA	1:E:25:SER:OG	2.11	0.51
1:E:197:THR:O	1:E:197:THR:CG2	2.59	0.51
1:A:113:MSE:HE3	1:A:181:ARG:NE	2.26	0.50
1:A:316:ARG:O	1:A:320:ASN:ND2	2.45	0.50
1:E:688:GLU:N	1:E:688:GLU:OE1	2.44	0.50
1:C:197:THR:O	1:C:197:THR:CG2	2.59	0.50
1:F:684:GLY:HA3	1:F:734:LYS:HB2	1.93	0.50
1:C:273:ARG:HB2	5:C:1009:HOH:O	2.10	0.50
1:D:456:ALA:O	1:D:457:ASP:HB3	2.12	0.50
1:A:268:VAL:C	1:A:269:LEU:HD12	2.31	0.50
1:B:122:GLU:O	1:B:126:GLU:HG3	2.11	0.50
1:D:120:MSE:HE3	1:D:226:VAL:CG2	2.40	0.50
1:B:22:GLU:O	1:B:26:VAL:HG23	2.12	0.50
1:B:74:ALA:HA	1:B:91:MSE:HG3	1.92	0.50
1:B:294:ASN:C	1:B:294:ASN:ND2	2.64	0.50
1:B:865:GLU:O	1:B:869:GLN:HG3	2.12	0.50
1:C:502:THR:HG23	1:C:887:LEU:HD21	1.94	0.50
1:E:120:MSE:HE1	1:E:123:ILE:HD11	1.93	0.50
1:C:208:LEU:HD22	1:D:208:LEU:HD22	1.94	0.50
1:F:120:MSE:CE	1:F:266:ALA:HB1	2.41	0.50
1:B:186:LEU:N	1:B:186:LEU:HD23	2.26	0.50
1:F:703:ILE:O	1:F:798:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:N	1:B:452:GLU:OE1	2.33	0.49
1:C:705:SER:CB	1:C:799:VAL:HB	2.42	0.49
1:E:590:ALA:N	1:E:591:PRO:HD2	2.26	0.49
1:F:303:THR:HA	1:F:441:ILE:O	2.12	0.49
1:B:12:LEU:HD12	1:B:15:TYR:CD2	2.46	0.49
1:C:74:ALA:HA	1:C:91:MSE:HG3	1.94	0.49
1:C:146:PHE:HD2	1:C:193:MSE:HE2	1.77	0.49
1:F:636:ALA:HB3	1:F:813:PHE:HE1	1.78	0.49
1:F:769:ASP:OD1	1:F:769:ASP:N	2.45	0.49
1:A:112:ALA:HB2	1:A:165:VAL:CG2	2.42	0.49
1:B:238:PHE:O	1:B:241:GLN:O	2.29	0.49
1:B:329:ASP:OD1	1:B:329:ASP:N	2.44	0.49
1:D:112:ALA:HB2	1:D:165:VAL:HG22	1.94	0.49
1:F:112:ALA:HB2	1:F:165:VAL:HG22	1.94	0.49
1:F:680:MSE:HE3	1:F:715:ALA:HB2	1.95	0.49
1:C:119:ILE:O	1:C:123:ILE:HG12	2.12	0.49
1:D:358:ASP:OD2	1:D:360:ASP:HB3	2.13	0.49
1:F:74:ALA:HA	1:F:91:MSE:HG3	1.93	0.49
1:F:500:ARG:HB3	1:F:500:ARG:HH11	1.78	0.49
1:B:398:ARG:CG	1:B:420:SER:O	2.61	0.49
1:A:108:ARG:HD3	1:A:164:GLU:O	2.12	0.49
1:C:856:LEU:HD22	1:C:860:HIS:CE1	2.48	0.49
1:E:773:TYR:HA	1:E:780:PRO:HA	1.95	0.49
1:B:318:LEU:HD23	1:B:449:ILE:HD13	1.96	0.48
1:D:646:ILE:HG12	1:D:663:LEU:HD13	1.94	0.48
1:A:709:PRO:N	1:A:802:GLN:HE22	2.11	0.48
1:B:120:MSE:HE2	1:B:123:ILE:HD11	1.94	0.48
1:A:238:PHE:O	1:A:241:GLN:O	2.32	0.48
1:E:294:ASN:C	1:E:294:ASN:ND2	2.66	0.48
1:B:197:THR:O	1:B:197:THR:CG2	2.60	0.48
1:C:814:ASP:OD1	1:C:814:ASP:N	2.45	0.48
1:D:386:LYS:NZ	5:D:1001:HOH:O	2.39	0.48
1:B:125:TRP:CE2	1:B:135:PRO:HG2	2.49	0.48
1:C:611:ASP:HA	1:C:668:SER:HB2	1.94	0.48
1:C:627:LEU:HD22	1:C:859:PHE:CE2	2.49	0.48
1:D:357:ARG:HB2	1:D:415:ALA:HB2	1.95	0.48
1:E:120:MSE:HE3	1:E:226:VAL:HG13	1.95	0.48
1:E:245:ALA:HB2	1:E:259:GLY:O	2.13	0.48
1:C:294:ASN:C	1:C:294:ASN:ND2	2.66	0.48
1:C:703:ILE:O	1:C:798:GLN:HG3	2.14	0.48
1:E:193:MSE:CE	1:E:208:LEU:HD13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:GLY:HA3	5:A:1037:HOH:O	2.14	0.48
1:C:365:ILE:HD12	1:C:416:VAL:HG13	1.94	0.48
1:D:579:ALA:HB1	1:D:583:ARG:NH2	2.29	0.48
1:B:697:PHE:O	1:B:698:ALA:C	2.51	0.48
1:E:775:THR:O	1:E:799:VAL:O	2.31	0.48
1:F:568:ALA:O	1:F:572:LEU:HB2	2.14	0.48
1:A:375:THR:HG23	1:A:379:ALA:N	2.29	0.48
1:C:146:PHE:CD2	1:C:193:MSE:HE2	2.49	0.48
1:F:728:CYS:O	1:F:733:HIS:N	2.39	0.48
1:F:108:ARG:HD3	1:F:164:GLU:O	2.14	0.48
1:F:343:PRO:HA	1:F:409:ILE:HG12	1.96	0.48
1:E:206:LEU:HD21	1:E:288:LEU:HD13	1.95	0.47
1:E:296:ASP:HB2	1:E:306:SER:HB3	1.95	0.47
1:A:146:PHE:HD2	1:A:193:MSE:HE2	1.80	0.47
1:B:197:THR:HG23	1:B:444:THR:HB	1.96	0.47
1:A:186:LEU:HD23	1:A:186:LEU:N	2.29	0.47
1:A:589:LEU:HD23	1:A:661:ALA:HB1	1.96	0.47
1:D:7:MSE:HE1	1:D:15:TYR:CD2	2.49	0.47
1:B:475:ARG:HH11	1:B:475:ARG:CG	2.27	0.47
1:A:568:ALA:O	1:A:572:LEU:HB2	2.15	0.47
1:A:876:SER:N	1:A:877:PRO:CD	2.77	0.47
1:B:471:VAL:CG2	1:B:867:TYR:CE2	2.97	0.47
1:B:562:ALA:HB1	1:B:821:PRO:HD2	1.97	0.47
1:F:663:LEU:HD11	1:F:791:TRP:CE2	2.50	0.47
1:A:197:THR:HG22	1:A:200:SER:OG	2.14	0.47
1:A:728:CYS:HB3	1:A:733:HIS:HB2	1.96	0.47
1:C:206:LEU:HD23	1:C:206:LEU:C	2.35	0.47
1:D:365:ILE:HD12	1:D:416:VAL:HG13	1.95	0.47
1:E:240:SER:C	1:E:241:GLN:O	2.50	0.47
1:E:566:GLY:O	1:E:567:MSE:C	2.51	0.47
1:F:375:THR:HG23	1:F:379:ALA:N	2.29	0.47
1:B:642:SER:OG	1:B:643:GLN:N	2.46	0.47
1:B:745:HIS:HA	1:B:796:ARG:O	2.14	0.47
1:C:627:LEU:HD22	1:C:859:PHE:CZ	2.50	0.47
1:B:384:VAL:O	1:B:388:VAL:HG23	2.15	0.47
1:C:120:MSE:HE1	1:C:266:ALA:HB1	1.96	0.47
1:E:46:MSE:CE	1:E:385:MSE:HG2	2.45	0.47
1:A:196:ASP:OD2	1:B:175:SER:HB3	2.15	0.47
1:E:771:ALA:HA	5:E:987:HOH:O	2.14	0.47
1:F:197:THR:CG2	1:F:200:SER:OG	2.63	0.47
1:F:697:PHE:O	1:F:698:ALA:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:VAL:HB	1:C:541:ARG:HB3	1.97	0.46
1:C:560:GLN:HE21	2:C:950:ACT:C	2.28	0.46
1:A:320:ASN:N	1:A:320:ASN:ND2	2.60	0.46
1:A:475:ARG:HG3	1:A:475:ARG:HH11	1.79	0.46
1:B:560:GLN:NE2	1:B:643:GLN:HE22	2.13	0.46
1:C:476:ASP:OD1	1:C:476:ASP:C	2.54	0.46
1:F:839:ALA:O	1:F:840:ASP:CB	2.63	0.46
1:A:12:LEU:N	1:A:12:LEU:HD23	2.31	0.46
1:D:863:LEU:HD22	1:D:873:VAL:CG1	2.45	0.46
1:A:586:GLU:OE1	1:A:598:THR:OG1	2.26	0.46
1:E:193:MSE:HE3	1:E:208:LEU:HD13	1.97	0.46
1:F:206:LEU:HD23	1:F:206:LEU:O	2.16	0.46
1:C:193:MSE:HE1	1:D:208:LEU:HD21	1.98	0.46
1:E:119:ILE:O	1:E:123:ILE:HG12	2.16	0.46
1:E:123:ILE:CD1	1:E:268:VAL:HG23	2.46	0.46
1:B:642:SER:OG	2:B:950:ACT:C	2.58	0.46
1:B:710:ARG:HG2	1:B:710:ARG:O	2.15	0.46
1:E:343:PRO:HA	1:E:409:ILE:HG12	1.98	0.46
1:D:207:HIS:ND1	1:D:291:SER:OG	2.48	0.46
1:D:567:MSE:O	1:D:568:ALA:HB3	2.15	0.46
1:E:125:TRP:CE2	1:E:135:PRO:HG2	2.51	0.46
1:F:114:ASP:OD2	1:F:152:VAL:HG13	2.15	0.46
1:A:303:THR:HA	1:A:441:ILE:O	2.16	0.45
1:B:120:MSE:CE	1:B:266:ALA:HB1	2.46	0.45
1:D:363:LEU:O	1:D:416:VAL:HA	2.16	0.45
1:A:697:PHE:O	1:A:698:ALA:C	2.54	0.45
1:B:175:SER:OG	1:B:194:THR:HG21	2.16	0.45
1:B:349:LEU:HD13	1:B:365:ILE:HD11	1.98	0.45
1:C:268:VAL:O	1:C:269:LEU:HD12	2.16	0.45
1:D:566:GLY:O	1:D:567:MSE:O	2.34	0.45
1:F:140:GLY:HA2	1:F:189:GLU:OE2	2.16	0.45
1:F:839:ALA:O	1:F:840:ASP:HB2	2.16	0.45
1:B:241:GLN:HE21	1:B:241:GLN:CA	2.28	0.45
1:D:475:ARG:HH11	1:D:475:ARG:CG	2.27	0.45
1:F:560:GLN:HG2	2:F:950:ACT:H1	1.97	0.45
1:F:740:VAL:HG22	1:F:742:TYR:CE1	2.50	0.45
1:B:82:PRO:HA	5:B:997:HOH:O	2.16	0.45
1:C:518:VAL:HG21	1:C:864:GLY:HA2	1.98	0.45
1:E:502:THR:HG23	1:E:887:LEU:HD21	1.98	0.45
1:A:772:LEU:HD12	1:A:772:LEU:C	2.37	0.45
1:D:120:MSE:CE	1:D:123:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:MSE:SE	1:E:226:VAL:HG22	2.66	0.45
1:F:186:LEU:HB2	1:F:188:LEU:HG	1.99	0.45
1:F:753:ARG:HG2	1:F:757:LEU:HD12	1.98	0.45
1:F:478:GLN:HG2	1:F:893:GLN:OE1	2.16	0.45
1:A:165:VAL:O	1:A:165:VAL:HG13	2.17	0.45
1:A:567:MSE:O	1:A:568:ALA:HB3	2.17	0.45
1:B:117:GLN:HG2	1:B:178:ALA:HA	1.99	0.45
1:D:608:ASP:OD1	1:D:608:ASP:N	2.49	0.45
1:E:186:LEU:N	1:E:186:LEU:HD23	2.31	0.45
1:B:197:THR:HG22	1:B:200:SER:OG	2.17	0.45
1:B:838:PRO:HB2	1:B:841:ALA:HB3	1.99	0.45
1:A:146:PHE:CD2	1:A:193:MSE:HE2	2.52	0.45
1:B:300:ASN:ND2	1:B:300:ASN:H	2.14	0.45
1:D:225:GLY:O	1:D:266:ALA:HA	2.17	0.45
1:B:705:SER:CB	1:B:799:VAL:HB	2.46	0.45
1:F:801:PHE:CZ	1:F:825:LEU:HD13	2.52	0.45
1:A:381:VAL:O	1:A:385:MSE:HG3	2.17	0.44
1:C:686:GLY:O	1:C:687:THR:C	2.55	0.44
1:E:342:ASP:HB2	1:E:343:PRO:HD3	1.99	0.44
1:C:123:ILE:HD12	1:C:268:VAL:HG23	1.98	0.44
1:C:705:SER:HA	1:C:799:VAL:HB	1.99	0.44
1:E:111:LEU:HA	1:E:897:TYR:HB3	2.00	0.44
1:F:641:HIS:O	1:F:644:GLY:N	2.49	0.44
1:B:294:ASN:ND2	1:B:445:ASN:HB2	2.32	0.44
1:C:197:THR:HG21	1:C:204:THR:OG1	2.18	0.44
1:D:119:ILE:O	1:D:123:ILE:HG12	2.17	0.44
1:D:301:GLY:O	1:D:302:LEU:C	2.55	0.44
1:E:268:VAL:O	1:E:269:LEU:HD12	2.17	0.44
1:E:475:ARG:HD2	1:E:513:TRP:CD2	2.52	0.44
1:F:98:PHE:CD1	1:F:118:ARG:HB3	2.52	0.44
1:C:125:TRP:CE2	1:C:135:PRO:HG2	2.52	0.44
1:E:177:VAL:HG22	1:F:442:SER:HB3	1.99	0.44
1:E:475:ARG:HD2	1:E:513:TRP:CE3	2.53	0.44
1:E:618:PHE:O	1:E:622:VAL:HG23	2.17	0.44
1:A:368:VAL:HG13	1:A:386:LYS:HD2	1.99	0.44
1:A:731:GLU:O	1:A:732:ALA:HB3	2.17	0.44
1:B:268:VAL:O	1:B:269:LEU:HD12	2.18	0.44
1:B:669:ARG:HG2	1:B:672:ARG:NH1	2.32	0.44
1:C:163:ASP:CB	1:C:166:LEU:HD12	2.48	0.44
1:D:206:LEU:HD21	1:D:288:LEU:HD13	1.99	0.44
1:D:268:VAL:O	1:D:269:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:VAL:O	1:D:615:PRO:HD2	2.18	0.44
1:F:122:GLU:O	1:F:126:GLU:HG3	2.16	0.44
1:A:46:MSE:CE	1:A:269:LEU:HD11	2.48	0.44
1:B:398:ARG:HG3	1:B:420:SER:O	2.16	0.44
1:D:74:ALA:HA	1:D:91:MSE:HG3	1.99	0.44
1:E:94:ALA:HB1	1:E:97:ASP:CG	2.38	0.44
1:A:318:LEU:HD23	1:A:449:ILE:HD13	2.00	0.44
1:C:686:GLY:O	1:C:688:GLU:N	2.51	0.44
1:D:564:TRP:O	1:D:567:MSE:HG2	2.18	0.44
1:B:856:LEU:HD22	1:B:860:HIS:CE1	2.52	0.44
1:C:799:VAL:HG13	5:C:1018:HOH:O	2.17	0.44
1:A:475:ARG:HD2	1:A:513:TRP:CD2	2.53	0.43
1:B:478:GLN:NE2	1:B:893:GLN:OE1	2.50	0.43
1:D:522:ASP:OD1	1:D:522:ASP:C	2.56	0.43
1:E:175:SER:HB3	1:F:196:ASP:OD2	2.17	0.43
1:E:294:ASN:ND2	1:E:445:ASN:HB2	2.33	0.43
1:F:294:ASN:HD21	1:F:445:ASN:HB2	1.83	0.43
1:A:44:VAL:HG13	1:A:131:ALA:HB1	2.00	0.43
1:A:120:MSE:HE1	1:A:266:ALA:HB1	2.00	0.43
1:A:123:ILE:HD12	1:A:268:VAL:HG23	2.00	0.43
1:A:375:THR:HG22	1:A:379:ALA:HA	2.00	0.43
1:B:238:PHE:HA	1:B:241:GLN:HE22	1.83	0.43
1:C:375:THR:HG23	1:C:379:ALA:N	2.33	0.43
1:A:663:LEU:HD11	1:A:791:TRP:CE2	2.53	0.43
1:C:120:MSE:HE3	1:C:226:VAL:CG1	2.43	0.43
1:A:125:TRP:CE2	1:A:135:PRO:HG2	2.53	0.43
1:D:380:GLY:O	1:D:384:VAL:HG23	2.18	0.43
1:F:567:MSE:O	1:F:568:ALA:HB3	2.17	0.43
1:A:511:SER:HB2	1:A:513:TRP:CE2	2.53	0.43
1:B:612:VAL:O	1:B:615:PRO:HD2	2.18	0.43
1:C:511:SER:HB2	1:C:513:TRP:CE2	2.53	0.43
1:D:494:GLU:HA	1:D:494:GLU:OE1	2.17	0.43
1:E:165:VAL:HG11	1:E:899:LEU:HD11	2.01	0.43
1:E:268:VAL:C	1:E:269:LEU:HD12	2.39	0.43
1:F:639:VAL:HG21	1:F:808:LEU:HD11	1.99	0.43
1:D:151:THR:HG23	1:D:151:THR:O	2.19	0.43
1:D:282:ARG:HB3	1:D:283:PRO:HD2	2.00	0.43
1:A:46:MSE:HE3	1:A:269:LEU:HG	2.01	0.43
1:B:689:GLN:HE22	1:B:693:ARG:NH1	2.16	0.43
1:D:200:SER:O	1:D:201:SER:C	2.56	0.43
1:F:46:MSE:HE2	1:F:269:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:641:HIS:O	1:F:642:SER:C	2.57	0.43
1:F:865:GLU:O	1:F:869:GLN:HG3	2.18	0.43
1:A:728:CYS:O	1:A:732:ALA:N	2.52	0.43
1:D:10:GLU:OE1	1:D:10:GLU:N	2.44	0.43
1:D:186:LEU:HB2	1:D:188:LEU:HG	2.01	0.43
1:F:509:ARG:NH2	1:F:884:PRO:HG3	2.34	0.43
1:A:120:MSE:SE	1:A:226:VAL:HG22	2.69	0.43
1:A:473:SER:HA	1:A:515:HIS:O	2.19	0.43
1:A:837:LEU:O	1:A:838:PRO:C	2.57	0.43
1:C:475:ARG:NE	1:C:513:TRP:CE3	2.87	0.43
1:D:558:PRO:HB3	1:D:825:LEU:HD12	2.01	0.43
1:F:125:TRP:CE2	1:F:135:PRO:HG2	2.54	0.43
1:F:307:GLY:N	1:F:308:PRO:CD	2.82	0.42
1:B:238:PHE:HB3	1:B:244:LEU:HG	2.01	0.42
1:C:628:TRP:CZ3	1:C:863:LEU:HD23	2.54	0.42
1:F:615:PRO:O	1:F:618:PHE:HB3	2.19	0.42
1:B:125:TRP:CH2	1:B:135:PRO:HB2	2.54	0.42
1:F:684:GLY:CA	1:F:734:LYS:HB2	2.50	0.42
1:A:620:VAL:HG11	1:A:821:PRO:HG3	2.01	0.42
1:A:880:ALA:O	1:A:881:ASP:HB2	2.20	0.42
1:B:663:LEU:HD11	1:B:791:TRP:CE2	2.55	0.42
1:B:689:GLN:HE21	1:B:689:GLN:HA	1.84	0.42
1:E:529:GLY:O	1:E:533:VAL:HG23	2.20	0.42
1:F:662:LYS:O	1:F:663:LEU:C	2.58	0.42
1:B:398:ARG:HG2	1:B:420:SER:O	2.19	0.42
1:C:568:ALA:O	1:C:572:LEU:HB2	2.20	0.42
1:D:143:THR:HG23	1:D:220:LEU:HB3	2.01	0.42
1:B:40:PRO:HB3	1:B:287:VAL:CG1	2.50	0.42
1:C:758:THR:HG22	1:C:759:GLU:N	2.34	0.42
1:D:120:MSE:HE3	1:D:226:VAL:CG1	2.48	0.42
1:E:867:TYR:HB2	1:E:873:VAL:HG21	2.02	0.42
1:F:145:VAL:O	1:F:192:ALA:HA	2.20	0.42
1:A:683:PHE:CZ	1:A:724:LEU:HD13	2.55	0.42
1:B:294:ASN:HD21	1:B:445:ASN:HB2	1.85	0.42
1:C:834:ASP:O	1:C:836:ALA:N	2.53	0.42
1:F:165:VAL:O	1:F:165:VAL:HG13	2.19	0.42
1:F:203:LEU:HD22	1:F:448:VAL:HG11	2.01	0.42
1:F:600:LEU:HD21	1:F:607:LEU:CD1	2.50	0.42
1:F:705:SER:HB3	1:F:799:VAL:HB	2.01	0.42
1:C:120:MSE:CE	1:C:123:ILE:HD11	2.49	0.42
1:C:143:THR:HG23	1:C:220:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:CYS:SG	1:F:385:MSE:HE1	2.60	0.42
1:D:694:ILE:HG12	1:D:701:LEU:HB2	2.01	0.42
1:E:499:LEU:N	3:E:975:SO4:O4	2.46	0.42
1:C:165:VAL:O	1:C:165:VAL:HG13	2.20	0.42
1:D:141:SER:O	1:D:142:ALA:HB3	2.20	0.42
1:D:491:LEU:HD12	1:D:491:LEU:HA	1.86	0.42
1:D:494:GLU:HG3	1:D:496:ARG:HB3	2.01	0.42
1:F:669:ARG:HG2	1:F:672:ARG:HH12	1.85	0.42
1:A:697:PHE:CD1	1:A:701:LEU:HD12	2.55	0.41
1:B:134:ASP:OD1	1:B:134:ASP:C	2.58	0.41
1:B:157:ARG:O	1:B:158:PRO:C	2.57	0.41
1:C:120:MSE:CE	1:C:266:ALA:HB1	2.50	0.41
1:E:863:LEU:HD22	1:E:873:VAL:CG1	2.49	0.41
1:A:375:THR:HG22	1:A:379:ALA:CA	2.50	0.41
1:B:708:GLY:C	1:B:802:GLN:NE2	2.74	0.41
1:C:186:LEU:N	1:C:186:LEU:HD23	2.36	0.41
1:C:297:GLY:HA2	1:D:188:LEU:O	2.20	0.41
1:F:363:LEU:O	1:F:416:VAL:HA	2.20	0.41
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.84	0.41
1:A:749:VAL:HG12	1:A:749:VAL:O	2.20	0.41
1:B:490:HIS:NE2	1:B:497:ASN:ND2	2.68	0.41
1:C:669:ARG:O	1:C:672:ARG:HB2	2.21	0.41
1:D:522:ASP:O	1:D:523:ARG:C	2.59	0.41
1:D:876:SER:HB2	1:D:877:PRO:HD3	2.02	0.41
1:F:134:ASP:OD1	1:F:134:ASP:C	2.58	0.41
1:C:120:MSE:HA	1:C:120:MSE:HE2	2.02	0.41
1:C:560:GLN:HE21	2:C:950:ACT:CH3	2.33	0.41
1:D:318:LEU:HD23	1:D:449:ILE:HD13	2.01	0.41
1:D:638:VAL:HG21	1:D:652:ALA:HB2	2.02	0.41
1:F:823:PRO:HD3	1:F:849:LEU:O	2.20	0.41
1:B:227:THR:O	1:B:264:GLU:HB2	2.20	0.41
1:D:303:THR:HA	1:D:441:ILE:O	2.21	0.41
1:E:120:MSE:HE3	1:E:226:VAL:HG22	2.01	0.41
1:E:697:PHE:O	1:E:698:ALA:C	2.59	0.41
1:F:113:MSE:HE2	1:F:118:ARG:HG2	2.03	0.41
1:E:522:ASP:O	1:E:523:ARG:C	2.57	0.41
1:F:318:LEU:HD23	1:F:449:ILE:HD13	2.02	0.41
1:B:307:GLY:N	1:B:308:PRO:CD	2.83	0.41
1:C:589:LEU:HD23	1:C:661:ALA:HB1	2.03	0.41
1:D:487:LEU:HA	1:D:487:LEU:HD13	1.82	0.41
1:C:112:ALA:HB2	1:C:165:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:MSE:SE	1:C:226:VAL:HG22	2.71	0.41
1:C:349:LEU:HD13	1:C:365:ILE:HD11	2.03	0.41
1:F:159:ASP:OD1	1:F:159:ASP:N	2.54	0.41
1:A:175:SER:HB3	1:B:196:ASP:OD2	2.20	0.41
1:A:582:ILE:HG23	1:A:597:LEU:HD13	2.03	0.41
1:B:120:MSE:SE	1:B:226:VAL:HG22	2.70	0.41
1:B:628:TRP:CZ3	1:B:863:LEU:HD23	2.56	0.41
1:C:134:ASP:OD2	1:C:511:SER:HA	2.21	0.41
1:C:560:GLN:NE2	2:C:950:ACT:C	2.84	0.41
1:C:671:LEU:HD13	1:C:795:LEU:HD11	2.02	0.41
1:D:125:TRP:CE2	1:D:135:PRO:HG2	2.55	0.41
1:E:639:VAL:CG2	1:E:808:LEU:HD11	2.50	0.41
1:F:685:LEU:HD22	1:F:689:GLN:HB3	2.02	0.41
1:F:744:SER:HB2	1:F:745:HIS:CD2	2.56	0.41
1:F:856:LEU:HD23	1:F:856:LEU:HA	1.92	0.41
1:A:590:ALA:N	1:A:591:PRO:HD2	2.36	0.41
1:B:511:SER:HB2	1:B:513:TRP:CE2	2.56	0.41
1:D:342:ASP:HB2	1:D:343:PRO:HD3	2.03	0.41
1:E:376:GLN:O	1:E:377:ALA:C	2.59	0.41
1:E:514:GLU:HB2	5:E:1012:HOH:O	2.21	0.41
1:F:46:MSE:HE2	1:F:269:LEU:HD11	2.02	0.41
1:A:294:ASN:HD21	1:A:445:ASN:HB2	1.85	0.40
1:C:291:SER:HB3	1:C:448:VAL:HG23	2.02	0.40
1:A:541:ARG:NH1	1:A:858:ASP:OD1	2.54	0.40
1:B:899:LEU:HA	1:B:900:PRO:HD3	1.87	0.40
1:D:819:VAL:O	1:D:819:VAL:HG12	2.21	0.40
1:E:206:LEU:HD23	1:E:206:LEU:C	2.42	0.40
1:C:688:GLU:O	1:C:692:GLU:CG	2.66	0.40
1:C:806:ARG:CZ	1:C:806:ARG:HB3	2.51	0.40
1:D:850:ARG:CG	1:D:851:ARG:N	2.85	0.40
1:A:122:GLU:O	1:A:126:GLU:HG3	2.21	0.40
1:A:696:ARG:HB3	5:A:988:HOH:O	2.20	0.40
1:B:475:ARG:HG2	1:B:890:TYR:OH	2.21	0.40
1:C:16:LEU:O	1:C:17:LYS:C	2.58	0.40
1:D:494:GLU:HG3	1:D:496:ARG:CB	2.52	0.40
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.97	0.40
1:A:838:PRO:HB2	1:A:841:ALA:HB3	2.04	0.40
1:B:491:LEU:HD12	1:B:491:LEU:HA	1.90	0.40
1:C:93:ALA:N	5:C:981:HOH:O	2.55	0.40
1:D:494:GLU:CD	1:D:495:PRO:HD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	876/917 (96%)	823 (94%)	43 (5%)	10 (1%)	12	21
1	B	876/917 (96%)	813 (93%)	55 (6%)	8 (1%)	14	27
1	C	876/917 (96%)	796 (91%)	69 (8%)	11 (1%)	10	17
1	D	876/917 (96%)	808 (92%)	58 (7%)	10 (1%)	12	21
1	E	871/917 (95%)	795 (91%)	65 (8%)	11 (1%)	10	17
1	F	870/917 (95%)	795 (91%)	61 (7%)	14 (2%)	8	13
All	All	5245/5502 (95%)	4830 (92%)	351 (7%)	64 (1%)	11	19

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ASP
1	A	567	MSE
1	B	403	ASP
1	B	698	ALA
1	C	687	THR
1	D	403	ASP
1	D	567	MSE
1	D	843	ALA
1	E	175	SER
1	E	403	ASP
1	E	523	ARG
1	E	698	ALA
1	E	843	ALA
1	F	360	ASP
1	F	416	VAL
1	F	567	MSE
1	A	698	ALA
1	B	240	SER
1	C	497	ASN
1	C	698	ALA

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Mol	Chain	Res	Type
1	C	758	THR
1	C	769	ASP
1	C	855	GLY
1	D	698	ALA
1	E	360	ASP
1	E	567	MSE
1	F	403	ASP
1	F	769	ASP
1	F	840	ASP
1	A	93	ALA
1	A	202	GLY
1	A	360	ASP
1	A	732	ALA
1	B	567	MSE
1	B	855	GLY
1	C	429	GLU
1	C	642	SER
1	C	835	SER
1	D	216	ASP
1	D	842	GLY
1	E	643	GLN
1	F	642	SER
1	F	855	GLY
1	A	335	GLY
1	B	800	ARG
1	D	242	GLY
1	A	416	VAL
1	A	900	PRO
1	B	838	PRO
1	C	416	VAL
1	C	493	ARG
1	D	416	VAL
1	D	496	ARG
1	E	376	GLN
1	E	416	VAL
1	F	24	ASP
1	F	826	THR
1	F	900	PRO
1	B	416	VAL
1	F	22	GLU
1	F	758	THR
1	E	900	PRO

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Mol	Chain	Res	Type
1	D	819	VAL
1	F	577	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	647/668 (97%)	558 (86%)	89 (14%)	3	4
1	B	650/668 (97%)	581 (89%)	69 (11%)	5	9
1	C	647/668 (97%)	571 (88%)	76 (12%)	4	7
1	D	652/668 (98%)	572 (88%)	80 (12%)	4	6
1	E	643/668 (96%)	579 (90%)	64 (10%)	6	11
1	F	638/668 (96%)	561 (88%)	77 (12%)	4	6
All	All	3877/4008 (97%)	3422 (88%)	455 (12%)	4	7

All (455) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LYS
1	A	18	ARG
1	A	23	LEU
1	A	29	ARG
1	A	31	ARG
1	A	36	ARG
1	A	44	VAL
1	A	46	MSE
1	A	49	ARG
1	A	92	LEU
1	A	165	VAL
1	A	166	LEU
1	A	171	THR
1	A	175	SER
1	A	179	SER

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Mol	Chain	Res	Type
1	A	186	LEU
1	A	226	VAL
1	A	249	ARG
1	A	258	ASP
1	A	268	VAL
1	A	289	ARG
1	A	294	ASN
1	A	306	SER
1	A	320	ASN
1	A	357	ARG
1	A	360	ASP
1	A	363	LEU
1	A	368	VAL
1	A	374	HIS
1	A	375	THR
1	A	419	VAL
1	A	430	ARG
1	A	433	ARG
1	A	437	SER
1	A	438	SER
1	A	441	ILE
1	A	457	ASP
1	A	471	VAL
1	A	475	ARG
1	A	487	LEU
1	A	494	GLU
1	A	509	ARG
1	A	511	SER
1	A	523	ARG
1	A	540	ASP
1	A	541	ARG
1	A	544	THR
1	A	548	ARG
1	A	551	ARG
1	A	563	GLN
1	A	572	LEU
1	A	583	ARG
1	A	597	LEU
1	A	600	LEU
1	A	607	LEU
1	A	610	VAL
1	A	617	LEU

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Mol	Chain	Res	Type
1	A	663	LEU
1	A	682	SER
1	A	685	LEU
1	A	689	GLN
1	A	696	ARG
1	A	706	VAL
1	A	712	VAL
1	A	724	LEU
1	A	734	LYS
1	A	736	ARG
1	A	740	VAL
1	A	741	ASP
1	A	750	GLU
1	A	763	ILE
1	A	769	ASP
1	A	772	LEU
1	A	775	THR
1	A	794	ASN
1	A	795	LEU
1	A	800	ARG
1	A	814	ASP
1	A	818	GLU
1	A	826	THR
1	A	834	ASP
1	A	835	SER
1	A	856	LEU
1	A	872	GLU
1	A	876	SER
1	A	885	VAL
1	A	889	VAL
1	A	899	LEU
1	B	12	LEU
1	B	14	ARG
1	B	15	TYR
1	B	18	ARG
1	B	29	ARG
1	B	151	THR
1	B	165	VAL
1	B	179	SER
1	B	186	LEU
1	B	206	LEU
1	B	212	SER

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Mol	Chain	Res	Type
1	B	226	VAL
1	B	241	GLN
1	B	268	VAL
1	B	289	ARG
1	B	294	ASN
1	B	300	ASN
1	B	306	SER
1	B	313	VAL
1	B	324	ARG
1	B	329	ASP
1	B	340	LEU
1	B	360	ASP
1	B	368	VAL
1	B	398	ARG
1	B	419	VAL
1	B	430	ARG
1	B	433	ARG
1	B	441	ILE
1	B	473	SER
1	B	475	ARG
1	B	477	GLU
1	B	487	LEU
1	B	491	LEU
1	B	511	SER
1	B	541	ARG
1	B	544	THR
1	B	548	ARG
1	B	563	GLN
1	B	593	VAL
1	B	597	LEU
1	B	600	LEU
1	B	607	LEU
1	B	608	ASP
1	B	617	LEU
1	B	630	SER
1	B	658	GLU
1	B	663	LEU
1	B	685	LEU
1	B	689	GLN
1	B	712	VAL
1	B	724	LEU
1	B	734	LYS

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Mol	Chain	Res	Type
1	B	740	VAL
1	B	741	ASP
1	B	746	SER
1	B	750	GLU
1	B	753	ARG
1	B	772	LEU
1	B	794	ASN
1	B	795	LEU
1	B	800	ARG
1	B	803	ASP
1	B	818	GLU
1	B	872	GLU
1	B	885	VAL
1	B	886	GLU
1	B	899	LEU
1	B	900	PRO
1	C	10	GLU
1	C	18	ARG
1	C	20	VAL
1	C	29	ARG
1	C	31	ARG
1	C	41	ILE
1	C	49	ARG
1	C	92	LEU
1	C	97	ASP
1	C	159	ASP
1	C	164	GLU
1	C	165	VAL
1	C	171	THR
1	C	200	SER
1	C	226	VAL
1	C	231	SER
1	C	240	SER
1	C	268	VAL
1	C	289	ARG
1	C	294	ASN
1	C	327	ASP
1	C	340	LEU
1	C	357	ARG
1	C	358	ASP
1	C	360	ASP
1	C	368	VAL

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Mol	Chain	Res	Type
1	C	375	THR
1	C	419	VAL
1	C	424	SER
1	C	430	ARG
1	C	433	ARG
1	C	437	SER
1	C	441	ILE
1	C	471	VAL
1	C	475	ARG
1	C	511	SER
1	C	525	GLU
1	C	541	ARG
1	C	544	THR
1	C	550	ARG
1	C	551	ARG
1	C	563	GLN
1	C	570	ASP
1	C	572	LEU
1	C	583	ARG
1	C	597	LEU
1	C	600	LEU
1	C	607	LEU
1	C	617	LEU
1	C	627	LEU
1	C	658	GLU
1	C	663	LEU
1	C	685	LEU
1	C	687	THR
1	C	689	GLN
1	C	696	ARG
1	C	706	VAL
1	C	712	VAL
1	C	724	LEU
1	C	734	LYS
1	C	736	ARG
1	C	740	VAL
1	C	750	GLU
1	C	759	GLU
1	C	769	ASP
1	C	772	LEU
1	C	775	THR
1	C	795	LEU

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Mol	Chain	Res	Type
1	C	800	ARG
1	C	803	ASP
1	C	826	THR
1	C	844	CYS
1	C	872	GLU
1	C	889	VAL
1	C	896	ARG
1	C	899	LEU
1	D	8	THR
1	D	12	LEU
1	D	16	LEU
1	D	17	LYS
1	D	23	LEU
1	D	30	LEU
1	D	31	ARG
1	D	44	VAL
1	D	46	MSE
1	D	49	ARG
1	D	97	ASP
1	D	164	GLU
1	D	165	VAL
1	D	166	LEU
1	D	171	THR
1	D	175	SER
1	D	226	VAL
1	D	247	ASP
1	D	268	VAL
1	D	289	ARG
1	D	294	ASN
1	D	306	SER
1	D	324	ARG
1	D	340	LEU
1	D	356	GLU
1	D	361	ASP
1	D	365	ILE
1	D	368	VAL
1	D	398	ARG
1	D	419	VAL
1	D	424	SER
1	D	430	ARG
1	D	433	ARG
1	D	441	ILE

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Mol	Chain	Res	Type
1	D	468	VAL
1	D	471	VAL
1	D	475	ARG
1	D	491	LEU
1	D	494	GLU
1	D	541	ARG
1	D	548	ARG
1	D	549	THR
1	D	550	ARG
1	D	551	ARG
1	D	563	GLN
1	D	572	LEU
1	D	593	VAL
1	D	597	LEU
1	D	600	LEU
1	D	607	LEU
1	D	608	ASP
1	D	617	LEU
1	D	627	LEU
1	D	639	VAL
1	D	663	LEU
1	D	669	ARG
1	D	682	SER
1	D	685	LEU
1	D	689	GLN
1	D	696	ARG
1	D	706	VAL
1	D	712	VAL
1	D	724	LEU
1	D	734	LYS
1	D	736	ARG
1	D	740	VAL
1	D	750	GLU
1	D	769	ASP
1	D	772	LEU
1	D	795	LEU
1	D	800	ARG
1	D	810	GLU
1	D	835	SER
1	D	840	ASP
1	D	844	CYS
1	D	858	ASP

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Mol	Chain	Res	Type
1	D	869	GLN
1	D	872	GLU
1	D	883	ARG
1	D	889	VAL
1	E	18	ARG
1	E	23	LEU
1	E	30	LEU
1	E	44	VAL
1	E	46	MSE
1	E	49	ARG
1	E	85	ASP
1	E	92	LEU
1	E	159	ASP
1	E	165	VAL
1	E	166	LEU
1	E	171	THR
1	E	200	SER
1	E	212	SER
1	E	226	VAL
1	E	240	SER
1	E	251	LYS
1	E	273	ARG
1	E	289	ARG
1	E	294	ASN
1	E	306	SER
1	E	324	ARG
1	E	340	LEU
1	E	352	THR
1	E	360	ASP
1	E	368	VAL
1	E	423	ARG
1	E	430	ARG
1	E	433	ARG
1	E	441	ILE
1	E	471	VAL
1	E	491	LEU
1	E	525	GLU
1	E	541	ARG
1	E	542	THR
1	E	548	ARG
1	E	550	ARG
1	E	563	GLN

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Mol	Chain	Res	Type
1	E	572	LEU
1	E	593	VAL
1	E	597	LEU
1	E	600	LEU
1	E	617	LEU
1	E	627	LEU
1	E	639	VAL
1	E	663	LEU
1	E	685	LEU
1	E	692	GLU
1	E	696	ARG
1	E	706	VAL
1	E	712	VAL
1	E	734	LYS
1	E	741	ASP
1	E	750	GLU
1	E	753	ARG
1	E	769	ASP
1	E	772	LEU
1	E	795	LEU
1	E	800	ARG
1	E	844	CYS
1	E	872	GLU
1	E	876	SER
1	E	885	VAL
1	E	889	VAL
1	F	29	ARG
1	F	49	ARG
1	F	59	SER
1	F	92	LEU
1	F	151	THR
1	F	159	ASP
1	F	165	VAL
1	F	166	LEU
1	F	173	THR
1	F	176	SER
1	F	197	THR
1	F	226	VAL
1	F	231	SER
1	F	247	ASP
1	F	268	VAL
1	F	289	ARG

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Mol	Chain	Res	Type
1	F	294	ASN
1	F	306	SER
1	F	340	LEU
1	F	357	ARG
1	F	361	ASP
1	F	363	LEU
1	F	365	ILE
1	F	368	VAL
1	F	374	HIS
1	F	419	VAL
1	F	424	SER
1	F	430	ARG
1	F	433	ARG
1	F	437	SER
1	F	441	ILE
1	F	487	LEU
1	F	491	LEU
1	F	496	ARG
1	F	500	ARG
1	F	511	SER
1	F	535	ASP
1	F	540	ASP
1	F	541	ARG
1	F	544	THR
1	F	550	ARG
1	F	551	ARG
1	F	563	GLN
1	F	572	LEU
1	F	583	ARG
1	F	597	LEU
1	F	598	THR
1	F	600	LEU
1	F	607	LEU
1	F	609	ARG
1	F	617	LEU
1	F	627	LEU
1	F	663	LEU
1	F	669	ARG
1	F	685	LEU
1	F	688	GLU
1	F	696	ARG
1	F	706	VAL

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Mol	Chain	Res	Type
1	F	718	SER
1	F	724	LEU
1	F	734	LYS
1	F	736	ARG
1	F	740	VAL
1	F	769	ASP
1	F	772	LEU
1	F	780	PRO
1	F	795	LEU
1	F	800	ARG
1	F	803	ASP
1	F	814	ASP
1	F	818	GLU
1	F	826	THR
1	F	850	ARG
1	F	865	GLU
1	F	876	SER
1	F	889	VAL
1	F	899	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	320	ASN
1	A	445	ASN
1	A	689	GLN
1	A	748	GLN
1	A	802	GLN
1	B	241	GLN
1	B	294	ASN
1	B	300	ASN
1	B	445	ASN
1	B	483	GLN
1	B	497	ASN
1	B	560	GLN
1	B	689	GLN
1	B	802	GLN
1	B	860	HIS
1	C	294	ASN
1	C	320	ASN
1	C	334	HIS

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Mol	Chain	Res	Type
1	C	478	GLN
1	C	483	GLN
1	C	560	GLN
1	C	643	GLN
1	D	294	ASN
1	D	376	GLN
1	D	445	ASN
1	D	497	ASN
1	D	560	GLN
1	D	689	GLN
1	D	802	GLN
1	D	807	GLN
1	E	294	ASN
1	E	334	HIS
1	E	490	HIS
1	E	497	ASN
1	F	294	ASN
1	F	334	HIS
1	F	445	ASN
1	F	560	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	E	950	-	3,3,3	0.88	0	3,3,3	0.87	0
2	ACT	B	950	-	3,3,3	0.75	0	3,3,3	1.62	1 (33%)
2	ACT	C	950	-	3,3,3	0.82	0	3,3,3	1.24	0
2	ACT	A	950	-	3,3,3	0.90	0	3,3,3	1.62	1 (33%)
3	SO4	E	975	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	975	-	4,4,4	0.17	0	6,6,6	0.25	0
3	SO4	A	975	-	4,4,4	0.26	0	6,6,6	0.20	0
3	SO4	C	975	-	4,4,4	0.27	0	6,6,6	0.25	0
2	ACT	F	950	-	3,3,3	0.91	0	3,3,3	1.90	1 (33%)
3	SO4	F	975	-	4,4,4	0.27	0	6,6,6	0.41	0
2	ACT	D	950	-	3,3,3	0.80	0	3,3,3	2.13	2 (66%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	950	ACT	OXT-C-O	-2.67	112.12	122.03
2	D	950	ACT	OXT-C-CH3	2.61	126.00	115.05
2	D	950	ACT	OXT-C-O	-2.59	112.42	122.03
2	A	950	ACT	OXT-C-O	-2.06	114.39	122.03
2	B	950	ACT	OXT-C-CH3	2.05	123.64	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	950	ACT	1	0
2	B	950	ACT	2	0
2	C	950	ACT	4	0
3	E	975	SO4	1	0
3	B	975	SO4	1	0
2	F	950	ACT	1	0
2	D	950	ACT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	867/917 (94%)	0.59	38 (4%)	39	41	34, 67, 80, 94	0
1	B	867/917 (94%)	0.85	57 (6%)	26	28	46, 67, 80, 93	0
1	C	867/917 (94%)	0.81	57 (6%)	26	28	47, 67, 80, 93	0
1	D	868/917 (94%)	1.24	168 (19%)	4	5	48, 67, 80, 93	0
1	E	862/917 (94%)	0.87	71 (8%)	19	21	48, 67, 81, 93	0
1	F	859/917 (93%)	0.82	55 (6%)	27	29	48, 67, 80, 93	0
All	All	5190/5502 (94%)	0.86	446 (8%)	18	20	34, 67, 80, 94	0

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	20	VAL	10.9
1	E	16	LEU	6.3
1	D	716	GLY	5.6
1	D	495	PRO	5.5
1	D	743	ALA	4.8
1	D	720	PRO	4.7
1	D	711	SER	4.7
1	B	901	ILE	4.7
1	D	551	ARG	4.6
1	D	840	ASP	4.5
1	C	901	ILE	4.4
1	A	769	ASP	4.3
1	B	12	LEU	4.3
1	F	901	ILE	4.1
1	B	841	ALA	4.0
1	E	551	ARG	4.0
1	D	732	ALA	4.0
1	B	560	GLN	3.9
1	D	714	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	742	TYR	3.9
1	D	560	GLN	3.9
1	E	901	ILE	3.8
1	F	692	GLU	3.8
1	D	668	SER	3.7
1	F	456	ALA	3.6
1	D	715	ALA	3.6
1	D	30	LEU	3.6
1	B	421	GLN	3.6
1	E	733	HIS	3.6
1	D	23	LEU	3.5
1	D	298	ALA	3.5
1	D	681	ALA	3.5
1	D	691	ALA	3.5
1	E	415	ALA	3.5
1	C	359	PRO	3.5
1	A	403	ASP	3.5
1	D	356	GLU	3.5
1	D	728	CYS	3.5
1	D	640	GLY	3.5
1	E	290	GLY	3.5
1	E	881	ASP	3.4
1	D	16	LEU	3.4
1	D	683	PHE	3.3
1	E	732	ALA	3.3
1	D	657	LEU	3.3
1	C	90	GLY	3.3
1	D	686	GLY	3.3
1	C	441	ILE	3.3
1	D	601	LEU	3.3
1	F	403	ASP	3.3
1	D	748	GLN	3.2
1	D	697	PHE	3.2
1	D	375	THR	3.2
1	B	742	TYR	3.2
1	C	15	TYR	3.2
1	D	706	VAL	3.2
1	D	740	VAL	3.2
1	D	837	LEU	3.2
1	F	30	LEU	3.2
1	A	241	GLN	3.2
1	E	683	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	854	GLY	3.2
1	D	717	GLU	3.1
1	A	734	LYS	3.1
1	D	670	VAL	3.1
1	E	441	ILE	3.1
1	D	340	LEU	3.1
1	D	685	LEU	3.1
1	D	661	ALA	3.1
1	C	9	GLU	3.1
1	C	756	LEU	3.1
1	B	419	VAL	3.1
1	C	541	ARG	3.1
1	C	839	ALA	3.1
1	C	841	ALA	3.1
1	D	721	LEU	3.0
1	E	19	THR	3.0
1	E	497	ASN	3.0
1	D	27	THR	3.0
1	B	537	ARG	3.0
1	C	415	ALA	3.0
1	F	602	SER	3.0
1	F	415	ALA	3.0
1	D	421	GLN	3.0
1	B	838	PRO	3.0
1	C	595	TRP	2.9
1	D	694	ILE	2.9
1	E	21	THR	2.9
1	C	422	ALA	2.9
1	D	724	LEU	2.9
1	E	340	LEU	2.9
1	F	34	GLU	2.9
1	A	411	TRP	2.9
1	E	296	ASP	2.9
1	E	495	PRO	2.9
1	A	733	HIS	2.9
1	B	538	ILE	2.9
1	D	602	SER	2.9
1	D	338	THR	2.9
1	D	839	ALA	2.9
1	E	339	ARG	2.9
1	F	551	ARG	2.9
1	F	726	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	838	PRO	2.9
1	C	854	GLY	2.9
1	E	294	ASN	2.9
1	D	749	VAL	2.8
1	B	353	TYR	2.8
1	C	560	GLN	2.8
1	D	608	ASP	2.8
1	A	551	ARG	2.8
1	D	616	ALA	2.8
1	C	411	TRP	2.8
1	B	415	ALA	2.8
1	D	302	LEU	2.8
1	D	12	LEU	2.8
1	D	199	CYS	2.7
1	D	26	VAL	2.7
1	B	411	TRP	2.7
1	D	563	GLN	2.7
1	B	756	LEU	2.7
1	E	17	LYS	2.7
1	D	316	ARG	2.7
1	B	365	ILE	2.7
1	B	840	ASP	2.7
1	F	728	CYS	2.7
1	A	560	GLN	2.7
1	C	246	ALA	2.7
1	E	365	ILE	2.7
1	A	886	GLU	2.7
1	D	169	VAL	2.7
1	D	198	ALA	2.7
1	D	309	ALA	2.7
1	E	325	ALA	2.7
1	D	10	GLU	2.7
1	D	611	ASP	2.7
1	F	404	GLU	2.7
1	D	735	ALA	2.7
1	D	710	ARG	2.7
1	A	466	GLY	2.7
1	D	164	GLU	2.6
1	D	296	ASP	2.6
1	D	323	VAL	2.6
1	D	600	LEU	2.6
1	C	855	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	695	GLY	2.6
1	E	540	ASP	2.6
1	C	497	ASN	2.6
1	D	726	ALA	2.6
1	F	839	ALA	2.6
1	D	746	SER	2.6
1	F	595	TRP	2.6
1	B	360	ASP	2.6
1	E	419	VAL	2.6
1	D	901	ILE	2.6
1	D	594	ASP	2.6
1	E	293	VAL	2.6
1	A	415	ALA	2.6
1	D	13	ARG	2.6
1	D	37	ALA	2.6
1	D	590	ALA	2.6
1	A	494	GLU	2.5
1	C	671	LEU	2.5
1	A	608	ASP	2.5
1	B	359	PRO	2.5
1	C	540	ASP	2.5
1	F	252	PRO	2.5
1	F	608	ASP	2.5
1	D	689	GLN	2.5
1	D	707	ASN	2.5
1	D	713	VAL	2.5
1	D	817	VAL	2.5
1	A	800	ARG	2.5
1	D	493	ARG	2.5
1	D	851	ARG	2.5
1	F	689	GLN	2.5
1	D	95	ALA	2.5
1	F	730	ALA	2.5
1	C	733	HIS	2.5
1	D	297	GLY	2.5
1	D	738	ILE	2.5
1	F	171	THR	2.5
1	E	420	SER	2.5
1	B	250	CYS	2.5
1	D	558	PRO	2.5
1	C	580	ASP	2.5
1	D	403	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	577	VAL	2.5
1	F	398	ARG	2.5
1	F	611	ASP	2.5
1	C	320	ASN	2.5
1	B	652	ALA	2.5
1	F	732	ALA	2.5
1	C	538	ILE	2.5
1	D	449	ILE	2.5
1	D	38	GLY	2.5
1	D	566	GLY	2.5
1	D	64	VAL	2.5
1	D	293	VAL	2.5
1	E	215	ARG	2.5
1	E	840	ASP	2.5
1	D	733	HIS	2.5
1	F	734	LYS	2.5
1	D	204	THR	2.5
1	D	719	GLY	2.5
1	F	248	GLY	2.5
1	F	332	GLU	2.5
1	D	701	LEU	2.5
1	D	614	GLN	2.5
1	A	839	ALA	2.5
1	E	535	ASP	2.5
1	C	600	LEU	2.4
1	C	551	ARG	2.4
1	E	26	VAL	2.4
1	B	199	CYS	2.4
1	D	446	ALA	2.4
1	B	769	ASP	2.4
1	C	365	ILE	2.4
1	E	449	ILE	2.4
1	D	19	THR	2.4
1	C	496	ARG	2.4
1	D	357	ARG	2.4
1	D	430	ARG	2.4
1	B	416	VAL	2.4
1	D	836	ALA	2.4
1	E	743	ALA	2.4
1	D	412	ASP	2.4
1	B	653	GLY	2.4
1	D	404	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	818	GLU	2.4
1	B	340	LEU	2.4
1	B	850	ARG	2.4
1	D	195	VAL	2.4
1	F	683	PHE	2.4
1	C	449	ILE	2.4
1	D	355	ALA	2.4
1	B	337	GLY	2.4
1	B	375	THR	2.4
1	E	587	ARG	2.4
1	D	308	PRO	2.4
1	E	442	SER	2.4
1	F	422	ALA	2.4
1	F	690	ALA	2.4
1	A	742	TYR	2.4
1	D	679	GLY	2.4
1	E	603	GLY	2.4
1	C	53	ASP	2.4
1	E	852	ASP	2.4
1	F	540	ASP	2.4
1	A	692	GLU	2.3
1	F	837	LEU	2.3
1	D	736	ARG	2.3
1	B	706	VAL	2.3
1	D	253	PHE	2.3
1	D	547	ALA	2.3
1	E	839	ALA	2.3
1	A	524	ASP	2.3
1	B	159	ASP	2.3
1	B	403	ASP	2.3
1	F	23	LEU	2.3
1	C	587	ARG	2.3
1	A	169	VAL	2.3
1	A	416	VAL	2.3
1	B	427	ALA	2.3
1	D	442	SER	2.3
1	D	642	SER	2.3
1	D	698	ALA	2.3
1	F	562	ALA	2.3
1	E	335	GLY	2.3
1	D	794	ASN	2.3
1	D	825	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	ASP	2.3
1	E	171	THR	2.3
1	C	669	ARG	2.3
1	D	315	ARG	2.3
1	D	500	ARG	2.3
1	D	305	PRO	2.3
1	B	260	PHE	2.3
1	C	260	PHE	2.3
1	A	365	ILE	2.3
1	A	901	ILE	2.3
1	B	743	ALA	2.3
1	D	554	ALA	2.3
1	E	602	SER	2.3
1	B	716	GLY	2.3
1	A	601	LEU	2.3
1	A	15	TYR	2.3
1	D	677	GLN	2.3
1	E	855	GLY	2.3
1	C	544	THR	2.2
1	C	792	TYR	2.2
1	D	444	THR	2.2
1	D	687	THR	2.2
1	F	777	THR	2.2
1	C	403	ASP	2.2
1	D	852	ASP	2.2
1	F	412	ASP	2.2
1	B	733	HIS	2.2
1	C	766	VAL	2.2
1	D	610	VAL	2.2
1	D	613	VAL	2.2
1	E	577	VAL	2.2
1	F	26	VAL	2.2
1	F	313	VAL	2.2
1	F	449	ILE	2.2
1	E	880	ALA	2.2
1	F	355	ALA	2.2
1	D	363	LEU	2.2
1	E	685	LEU	2.2
1	A	583	ARG	2.2
1	D	299	SER	2.2
1	D	737	ARG	2.2
1	B	356	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	477	GLU	2.2
1	C	776	THR	2.2
1	C	330	TYR	2.2
1	D	445	ASN	2.2
1	D	419	VAL	2.2
1	E	368	VAL	2.2
1	C	646	ILE	2.2
1	D	365	ILE	2.2
1	A	841	ALA	2.2
1	C	660	ALA	2.2
1	D	604	ALA	2.2
1	F	37	ALA	2.2
1	B	435	GLY	2.2
1	F	90	GLY	2.2
1	B	237	GLU	2.2
1	F	32	GLU	2.2
1	C	338	THR	2.2
1	E	375	THR	2.2
1	D	570	ASP	2.2
1	E	24	ASP	2.2
1	F	840	ASP	2.2
1	E	538	ILE	2.2
1	A	257	ALA	2.2
1	E	730	ALA	2.2
1	D	262	LEU	2.2
1	D	572	LEU	2.2
1	D	589	LEU	2.2
1	E	23	LEU	2.2
1	E	350	LEU	2.2
1	B	242	GLY	2.2
1	B	466	GLY	2.2
1	B	561	GLY	2.2
1	C	89	GLY	2.2
1	D	290	GLY	2.2
1	D	573	ARG	2.2
1	D	850	ARG	2.2
1	E	398	ARG	2.2
1	E	466	GLY	2.2
1	C	291	SER	2.2
1	D	237	GLU	2.2
1	D	702	SER	2.2
1	F	162	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	402	PHE	2.2
1	D	260	PHE	2.2
1	B	837	LEU	2.2
1	C	244	LEU	2.2
1	D	415	ALA	2.2
1	B	62	GLU	2.1
1	B	900	PRO	2.1
1	C	429	GLU	2.1
1	F	84	PRO	2.1
1	B	179	SER	2.1
1	E	544	THR	2.1
1	E	323	VAL	2.1
1	D	607	LEU	2.1
1	D	752	LEU	2.1
1	F	413	LEU	2.1
1	A	732	ALA	2.1
1	C	37	ALA	2.1
1	D	178	ALA	2.1
1	D	312	ARG	2.1
1	D	609	ARG	2.1
1	E	440	GLY	2.1
1	D	727	GLU	2.1
1	B	744	SER	2.1
1	D	294	ASN	2.1
1	A	773	TYR	2.1
1	B	577	VAL	2.1
1	C	418	VAL	2.1
1	D	182	VAL	2.1
1	D	353	TYR	2.1
1	D	799	VAL	2.1
1	E	837	LEU	2.1
1	F	760	LEU	2.1
1	A	844	CYS	2.1
1	F	414	GLY	2.1
1	A	283	PRO	2.1
1	B	364	TRP	2.1
1	D	410	GLU	2.1
1	A	538	ILE	2.1
1	C	419	VAL	2.1
1	D	725	ILE	2.1
1	E	64	VAL	2.1
1	F	365	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	580	ASP	2.1
1	D	15	TYR	2.1
1	E	188	LEU	2.1
1	A	456	ALA	2.1
1	D	215	ARG	2.1
1	E	878	ALA	2.1
1	D	855	GLY	2.1
1	E	380	GLY	2.1
1	A	250	CYS	2.1
1	C	332	GLU	2.1
1	E	356	GLU	2.1
1	F	164	GLU	2.1
1	A	544	THR	2.1
1	D	744	SER	2.1
1	E	291	SER	2.1
1	E	799	VAL	2.1
1	E	445	ASN	2.1
1	C	737	ARG	2.1
1	D	741	ASP	2.1
1	B	246	ALA	2.1
1	B	148	GLY	2.1
1	F	62	GLU	2.0
1	B	347	HIS	2.0
1	D	544	THR	2.0
1	D	703	ILE	2.0
1	E	195	VAL	2.0
1	E	421	GLN	2.0
1	E	697	PHE	2.0
1	A	685	LEU	2.0
1	E	721	LEU	2.0
1	F	340	LEU	2.0
1	E	800	ARG	2.0
1	D	810	GLU	2.0
1	B	775	THR	2.0
1	B	795	LEU	2.0
1	D	33	VAL	2.0
1	D	165	VAL	2.0
1	D	166	LEU	2.0
1	E	376	GLN	2.0
1	A	36	ARG	2.0
1	C	442	SER	2.0
1	C	493	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	800	ARG	2.0
1	F	442	SER	2.0
1	B	588	ALA	2.0
1	B	732	ALA	2.0
1	C	174	ALA	2.0
1	C	611	ASP	2.0
1	E	258	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	975	5/5	0.73	0.15	109,109,109,109	0
3	SO4	E	975	5/5	0.80	0.17	101,101,102,102	5
3	SO4	C	975	5/5	0.82	0.17	84,84,85,86	5
4	CL	D	951	1/1	0.82	0.15	90,90,90,90	0
2	ACT	D	950	4/4	0.83	0.18	61,61,61,62	0
4	CL	F	976	1/1	0.87	0.15	76,76,76,76	0
2	ACT	F	950	4/4	0.88	0.16	44,44,45,45	0
4	CL	C	976	1/1	0.89	0.13	82,82,82,82	0
4	CL	E	976	1/1	0.92	0.12	70,70,70,70	0
2	ACT	B	950	4/4	0.92	0.15	50,50,50,50	0
3	SO4	A	975	5/5	0.93	0.18	87,87,88,88	0
2	ACT	A	950	4/4	0.93	0.15	51,51,51,51	0
2	ACT	E	950	4/4	0.94	0.14	47,48,48,48	0
2	ACT	C	950	4/4	0.94	0.13	54,54,54,54	0
3	SO4	F	975	5/5	0.95	0.19	82,82,83,83	0
4	CL	B	976	1/1	0.98	0.09	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.