



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 01:15 PM EDT

PDB ID : 3OQO
Title : Ccpa-hpr-ser46p-syn cre
Authors : schumacher, M.A.; Sprehe, M.; Bartholomae, M.; Hillen, W.; Brennan, R.G.
Deposited on : 2010-09-03
Resolution : 2.97 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

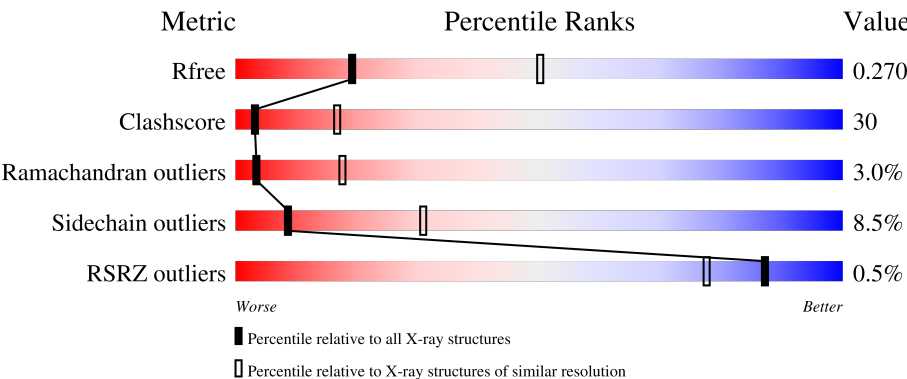
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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.



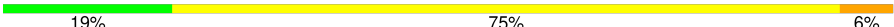
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

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	339	<div> <div>47%</div> <div>46%</div> <div>• •</div> </div>
1	C	339	<div> <div>45%</div> <div>48%</div> <div>• •</div> </div>
2	D	87	<div> <div>2%</div> <div>43%</div> <div>44%</div> <div>14%</div> </div>
2	S	87	<div> <div>44%</div> <div>45%</div> <div>11%</div> </div>
3	E	16	<div> <div>6%</div> <div>94%</div> </div>

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Mol	Chain	Length	Quality of chain
4	B	16	 A horizontal bar chart showing the quality of chain B. The bar is divided into three segments: a green segment on the left labeled '19%', a yellow segment in the middle labeled '75%', and a small orange segment on the right labeled '6%'.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7160 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 Catabolite control protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2584	1630	439	503	12			
1	C	332	Total	C	N	O	S	0	0	0
			2579	1627	438	502	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP P25144
A	336	HIS	-	expression tag	UNP P25144
A	337	HIS	-	expression tag	UNP P25144
A	338	HIS	-	expression tag	UNP P25144
A	339	HIS	-	expression tag	UNP P25144
A	340	HIS	-	expression tag	UNP P25144
C	335	HIS	-	expression tag	UNP P25144
C	336	HIS	-	expression tag	UNP P25144
C	337	HIS	-	expression tag	UNP P25144
C	338	HIS	-	expression tag	UNP P25144
C	339	HIS	-	expression tag	UNP P25144
C	340	HIS	-	expression tag	UNP P25144

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	S	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			
2	D	87	Total	C	N	O	P	S	0	0	0
			637	389	106	138	1	3			

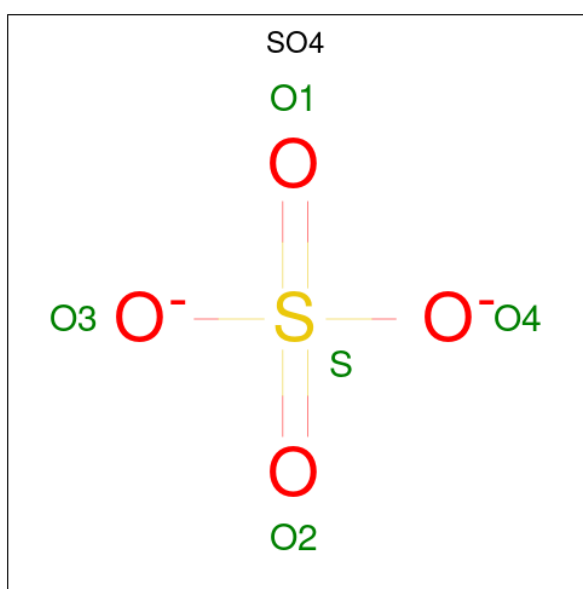
- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			

- Molecule 4 is a DNA chain called 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

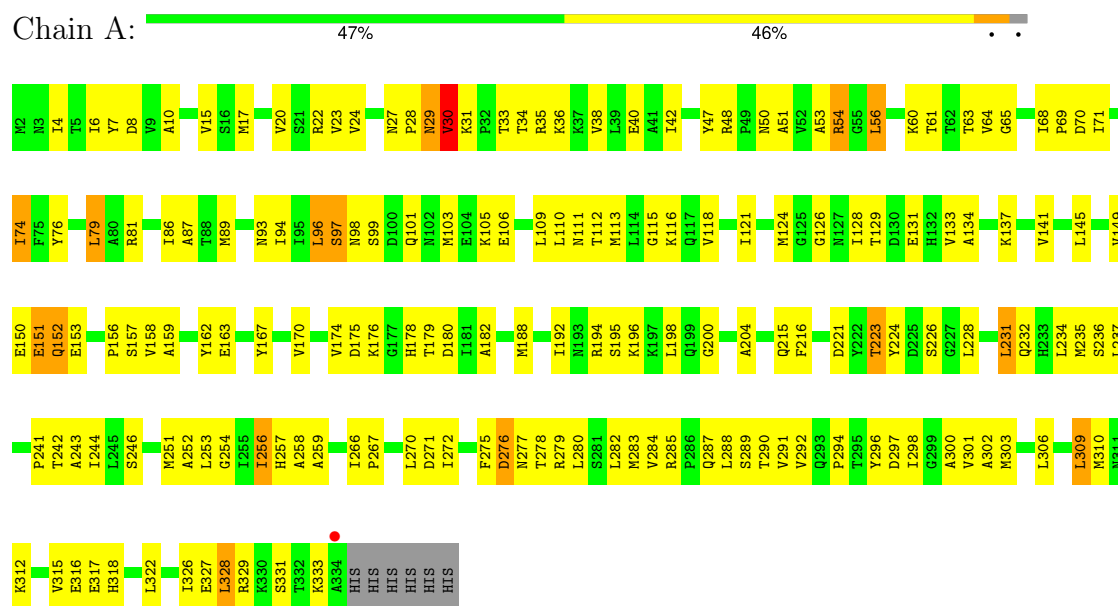
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total 23	O 23	0	0
6	S	8	Total 8	O 8	0	0
6	C	13	Total 13	O 13	0	0
6	E	2	Total 2	O 2	0	0
6	B	2	Total 2	O 2	0	0

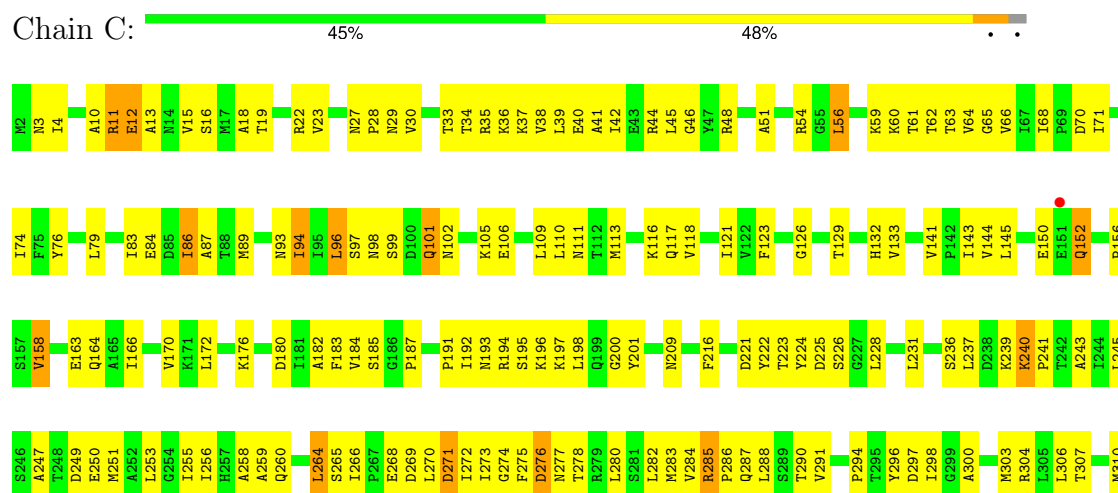
3 Residue-property plots

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: Catabolite control protein A

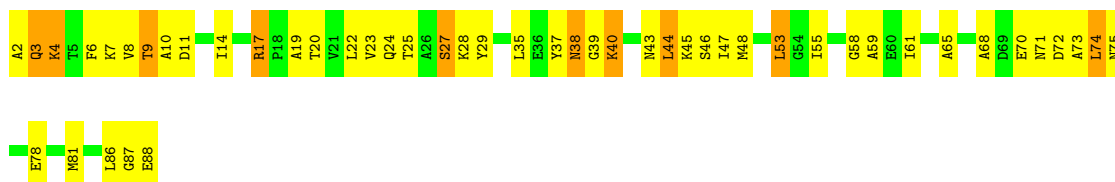


• Molecule 1: Catabolite control protein A

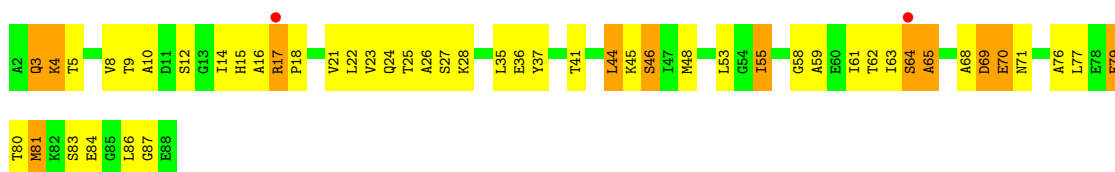




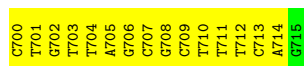
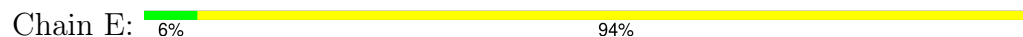
● Molecule 2: Phosphocarrier protein HPr



● Molecule 2: Phosphocarrier protein HPr



● Molecule 3: 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'



● Molecule 4: 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.15Å 105.21Å 173.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.40 – 2.97 56.40 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.0 (56.40-2.97) 99.0 (56.40-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.270 0.210 , 0.270	Depositor DCC
R_{free} test set	1959 reflections (6.87%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7160	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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, SEP

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	0.39	0/2624	0.62	0/3556
1	C	0.36	0/2619	0.59	0/3549
2	D	0.33	0/630	0.52	0/846
2	S	0.36	0/630	0.55	0/846
3	E	0.57	0/360	0.79	0/554
4	B	0.58	0/368	0.80	0/566
All	All	0.39	0/7231	0.62	0/9917

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
4	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	700	DC	Sidechain
4	B	713	DC	Sidechain

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	2584	0	2627	167	0
1	C	2579	0	2622	158	0
2	D	637	0	631	46	0
2	S	637	0	631	49	0
3	E	323	0	184	26	0
4	B	327	0	180	20	0
5	A	10	0	0	0	0
5	C	15	0	0	0	0
6	A	23	0	0	1	0
6	B	2	0	0	0	0
6	C	13	0	0	1	0
6	E	2	0	0	0	0
6	S	8	0	0	1	0
All	All	7160	0	6875	424	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 30.

All (424) 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)
3:E:710:DT:H2''	3:E:711:DT:H5'	1.17	1.16
2:D:9:THR:HG22	2:D:87:GLY:H	1.16	1.10
1:A:30:VAL:HG23	1:A:35:ARG:HH21	1.11	1.09
1:C:89:MET:HG3	2:D:24:GLN:HE21	1.16	1.09
1:A:23:VAL:HG21	1:A:38:VAL:HG11	1.44	0.97
1:A:71:ILE:HD11	1:C:71:ILE:HD11	1.48	0.96
1:C:30:VAL:HB	1:C:35:ARG:HH21	1.34	0.92
3:E:710:DT:H2''	3:E:711:DT:C5'	2.00	0.91
1:A:30:VAL:CG2	1:A:35:ARG:HH21	1.84	0.90
3:E:700:DC:HO5'	3:E:700:DC:H6	1.17	0.90
3:E:712:DT:H2''	3:E:713:DC:H5''	1.52	0.89
1:A:156:PRO:HB3	1:A:318:HIS:HB3	1.53	0.89
1:A:63:THR:HG22	1:A:93:ASN:HB2	1.55	0.89
2:S:17:ARG:HH21	2:S:17:ARG:HB2	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:703:DT:H3	4:B:712:DA:H2	1.21	0.87
3:E:713:DC:H2''	3:E:714:DA:C8	2.08	0.87
2:S:17:ARG:HB2	2:S:17:ARG:NH2	1.89	0.85
3:E:704:DT:H3	4:B:711:DA:H2	1.23	0.85
1:C:133:VAL:HG21	1:C:152:GLN:HG3	1.59	0.84
1:C:89:MET:HG3	2:D:24:GLN:NE2	1.91	0.84
1:A:288:LEU:HA	1:A:331:SER:HB2	1.60	0.82
1:C:70:ASP:HA	1:C:98:ASN:HD22	1.42	0.82
1:C:101:GLN:HE22	1:C:126:GLY:H	1.25	0.82
1:C:231:LEU:HB2	1:C:255:ILE:HG23	1.61	0.82
4:B:701:DT:H2''	4:B:702:DG:C8	2.14	0.82
1:A:182:ALA:HB3	1:A:244:ILE:HG23	1.61	0.80
1:C:156:PRO:HB3	1:C:318:HIS:HB3	1.64	0.80
1:A:30:VAL:HG23	1:A:35:ARG:NH2	1.95	0.79
1:C:86:ILE:HG22	1:C:303:MET:HG3	1.62	0.79
1:C:71:ILE:H	1:C:98:ASN:ND2	1.81	0.79
1:C:12:GLU:HG3	1:C:45:LEU:HD11	1.64	0.79
3:E:709:DC:H6	3:E:709:DC:H5'	1.47	0.78
1:C:19:THR:HG22	1:C:22:ARG:HH11	1.49	0.77
1:A:145:LEU:HB2	1:A:157:SER:CB	2.15	0.77
1:C:71:ILE:H	1:C:98:ASN:HD21	1.29	0.77
1:A:328:LEU:HD12	1:A:328:LEU:H	1.49	0.76
1:A:152:GLN:H	1:A:152:GLN:NE2	1.84	0.76
1:A:63:THR:HG23	1:C:116:LYS:HZ1	1.50	0.76
1:A:109:LEU:O	1:A:113:MET:HG3	1.86	0.76
1:C:59:LYS:O	1:C:60:LYS:HD2	1.86	0.76
1:A:68:ILE:HG13	1:A:124:MET:HE3	1.68	0.76
3:E:710:DT:C2'	3:E:711:DT:H5'	2.10	0.76
1:C:68:ILE:HD11	1:C:76:TYR:HB3	1.67	0.76
1:A:63:THR:HG23	1:C:116:LYS:NZ	2.02	0.75
1:A:133:VAL:HG21	1:A:152:GLN:HG3	1.69	0.75
2:S:27:SER:HA	2:S:45:LYS:HG2	1.68	0.75
1:A:231:LEU:HD11	1:A:259:ALA:HB2	1.69	0.75
1:A:256:ILE:HD11	1:A:272:ILE:HG21	1.66	0.74
2:D:9:THR:HG22	2:D:87:GLY:N	1.99	0.73
1:C:19:THR:CG2	1:C:22:ARG:HH11	2.01	0.73
1:C:118:VAL:HG21	1:C:121:ILE:HD11	1.68	0.73
1:C:23:VAL:HG21	1:C:38:VAL:HG11	1.71	0.72
3:E:708:DG:H1'	3:E:709:DC:H5''	1.71	0.70
2:D:17:ARG:O	2:D:21:VAL:HG23	1.92	0.70
1:A:71:ILE:CD1	1:C:71:ILE:HD11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:HG2	1:A:152:GLN:HG2	1.73	0.70
1:A:71:ILE:HD11	1:C:71:ILE:CD1	2.20	0.70
1:C:74:ILE:HD12	1:C:74:ILE:H	1.57	0.70
1:A:68:ILE:HD11	1:A:76:TYR:HB3	1.73	0.69
1:A:56:LEU:HD12	1:C:56:LEU:HD12	1.74	0.69
1:A:98:ASN:OD1	1:C:84:GLU:HG2	1.93	0.69
1:A:246:SER:HB3	1:A:252:ALA:HB2	1.75	0.69
1:C:56:LEU:HD22	4:B:707:DC:H1'	1.74	0.69
2:D:35:LEU:HB2	2:D:44:LEU:HD23	1.74	0.69
2:S:40:LYS:HD3	2:S:40:LYS:H	1.57	0.68
2:D:8:VAL:HG22	2:D:59:ALA:H	1.59	0.67
2:S:8:VAL:HG23	2:S:58:GLY:H	1.58	0.67
1:A:94:ILE:HD11	1:A:303:MET:HE3	1.76	0.67
1:C:102:ASN:HD22	1:C:105:LYS:H	1.40	0.67
1:A:294:PRO:HB2	1:A:297:ASP:HB2	1.77	0.67
1:C:264:LEU:HD23	1:C:264:LEU:H	1.60	0.67
1:C:30:VAL:HB	1:C:35:ARG:NH2	2.06	0.66
1:C:152:GLN:CD	1:C:152:GLN:H	1.98	0.66
1:A:159:ALA:HA	1:A:298:ILE:HD12	1.76	0.66
2:S:8:VAL:CG2	2:S:59:ALA:H	2.08	0.66
2:D:26:ALA:CB	2:D:44:LEU:HD12	2.27	0.65
1:C:129:THR:O	1:C:132:HIS:HB2	1.96	0.65
1:A:71:ILE:H	1:A:98:ASN:ND2	1.95	0.65
1:C:158:VAL:O	1:C:298:ILE:HG23	1.97	0.64
1:A:145:LEU:HB2	1:A:157:SER:HB2	1.79	0.64
1:A:20:VAL:O	1:A:24:VAL:HG23	1.98	0.64
1:C:126:GLY:O	1:C:191:PRO:HD2	1.97	0.64
1:A:231:LEU:CD1	1:A:259:ALA:HB2	2.29	0.63
2:D:14:ILE:HB	2:D:55:ILE:HB	1.79	0.63
1:A:42:ILE:HG23	1:A:47:TYR:HB3	1.82	0.62
1:A:145:LEU:HB2	1:A:157:SER:HB3	1.79	0.62
1:A:283:MET:HE3	1:C:250:GLU:HG3	1.79	0.62
1:C:253:LEU:HG	1:C:284:VAL:HG21	1.82	0.62
1:A:277:ASN:H	1:A:290:THR:HG21	1.64	0.62
1:C:166:ILE:O	1:C:170:VAL:HG23	1.98	0.62
1:A:134:ALA:HA	1:A:137:LYS:HE3	1.82	0.62
1:A:51:ALA:HB3	1:C:116:LYS:HA	1.82	0.61
2:D:81:MET:HE2	2:D:81:MET:HA	1.82	0.61
2:D:76:ALA:O	2:D:79:GLU:HB3	1.99	0.61
1:C:71:ILE:HG12	1:C:71:ILE:O	2.00	0.61
1:A:97:SER:HA	1:C:84:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TYR:HB2	1:A:17:MET:CE	2.31	0.61
1:A:277:ASN:N	1:A:290:THR:HG21	2.16	0.61
1:A:29:ASN:O	1:A:30:VAL:HG13	2.00	0.61
1:A:246:SER:CB	1:A:252:ALA:HB2	2.31	0.61
1:A:309:LEU:HD11	1:A:315:VAL:HG21	1.82	0.61
1:A:283:MET:CE	1:C:250:GLU:HG3	2.31	0.61
1:C:144:VAL:HG23	1:C:306:LEU:HD13	1.82	0.61
1:C:38:VAL:O	1:C:41:ALA:HB3	2.01	0.60
3:E:704:DT:H2''	3:E:705:DA:H5'	1.83	0.60
1:C:121:ILE:HB	1:C:143:ILE:HG12	1.84	0.60
1:A:54:ARG:HD2	1:A:54:ARG:O	2.01	0.60
1:A:116:LYS:HA	1:C:51:ALA:HB3	1.83	0.60
3:E:700:DC:H6	3:E:700:DC:O5'	1.83	0.60
1:A:36:LYS:O	1:A:40:GLU:HG2	2.01	0.60
1:C:278:THR:OG1	1:C:280:LEU:HB2	2.02	0.60
1:A:63:THR:CG2	1:C:116:LYS:HZ1	2.14	0.59
1:A:253:LEU:HD23	1:A:253:LEU:O	2.03	0.59
1:A:279:ARG:NH1	1:C:74:ILE:HD11	2.18	0.59
1:A:152:GLN:H	1:A:152:GLN:CD	2.04	0.59
2:S:25:THR:O	2:S:28:LYS:HG2	2.03	0.59
1:C:66:VAL:HB	1:C:96:LEU:HD22	1.84	0.59
1:C:276:ASP:HB3	1:C:278:THR:HG23	1.84	0.59
1:A:54:ARG:HD2	1:A:54:ARG:C	2.23	0.58
1:C:265:SER:HB3	1:C:268:GLU:HB2	1.85	0.58
1:A:68:ILE:HG13	1:A:124:MET:CE	2.34	0.57
2:S:10:ALA:HB2	2:S:86:LEU:HA	1.85	0.57
1:A:242:THR:O	1:A:270:LEU:HD12	2.04	0.57
1:A:271:ASP:C	1:A:272:ILE:HD12	2.23	0.57
1:A:275:PHE:O	1:A:276:ASP:HB2	2.03	0.57
1:C:66:VAL:HG21	1:C:94:ILE:HD13	1.85	0.57
1:A:179:THR:HG22	1:A:180:ASP:OD1	2.04	0.57
2:D:64:SER:O	2:D:65:ALA:HB2	2.05	0.57
1:C:41:ALA:O	1:C:45:LEU:HD13	2.05	0.57
4:B:704:DA:H1'	4:B:705:DA:H5'	1.87	0.57
1:C:183:PHE:CE1	1:C:185:SER:HB3	2.40	0.57
1:C:86:ILE:HG12	1:C:300:ALA:HB1	1.85	0.56
1:C:275:PHE:N	1:C:290:THR:HG23	2.20	0.56
2:S:4:LYS:NZ	2:S:78:GLU:OE2	2.37	0.56
3:E:709:DC:H5'	3:E:709:DC:C6	2.35	0.56
1:A:289:SER:H	1:A:331:SER:HB3	1.69	0.56
1:C:99:SER:HB2	1:C:106:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:VAL:HG13	2:D:44:LEU:O	2.06	0.56
1:A:56:LEU:HD22	3:E:707:DC:H1'	1.88	0.56
1:C:152:GLN:H	1:C:152:GLN:NE2	2.03	0.56
2:D:80:THR:HA	2:D:83:SER:HB2	1.87	0.56
1:A:294:PRO:O	1:A:298:ILE:HG12	2.06	0.56
1:C:275:PHE:CA	1:C:290:THR:HG23	2.35	0.56
1:C:83:ILE:HG22	1:C:94:ILE:HD11	1.87	0.56
1:C:256:ILE:HG22	1:C:260:GLN:OE1	2.05	0.56
1:C:71:ILE:HG22	1:C:98:ASN:HD21	1.71	0.55
1:C:275:PHE:HA	1:C:290:THR:HG23	1.88	0.55
2:S:37:TYR:O	2:S:38:ASN:C	2.45	0.55
1:A:223:THR:CG2	1:A:226:SER:H	2.20	0.55
2:S:37:TYR:HE2	2:S:59:ALA:HB1	1.72	0.55
1:C:223:THR:HG22	1:C:225:ASP:H	1.70	0.55
1:C:34:THR:O	1:C:37:LYS:HB3	2.05	0.55
2:S:3:GLN:O	2:S:4:LYS:HB2	2.07	0.55
1:C:182:ALA:HB2	1:C:241:PRO:HG2	1.87	0.55
4:B:702:DG:H2''	4:B:703:DA:C8	2.41	0.55
1:C:277:ASN:H	1:C:290:THR:HG21	1.71	0.55
1:A:290:THR:HG22	1:A:291:VAL:N	2.22	0.54
2:S:9:THR:HG21	2:S:88:GLU:HG3	1.88	0.54
1:C:269:ASP:O	1:C:270:LEU:HD12	2.07	0.54
1:A:7:TYR:HB2	1:A:17:MET:HE3	1.89	0.54
1:C:64:VAL:HG12	1:C:65:GLY:N	2.21	0.54
1:C:266:ILE:HD12	1:C:272:ILE:HD11	1.87	0.54
1:A:87:ALA:HB2	1:A:303:MET:CE	2.38	0.54
3:E:704:DT:N3	4:B:711:DA:H2	2.00	0.54
1:A:301:VAL:HG13	2:S:48:MET:HG2	1.90	0.54
1:C:311:ASN:HD22	1:C:313:GLU:HG2	1.73	0.54
2:D:63:ILE:HG21	2:D:77:LEU:HD13	1.88	0.54
1:A:68:ILE:O	1:A:98:ASN:HA	2.07	0.54
1:A:96:LEU:HD13	1:A:97:SER:N	2.23	0.54
1:A:167:TYR:CE1	1:A:204:ALA:HA	2.43	0.54
1:A:129:THR:O	1:A:133:VAL:HG23	2.07	0.53
2:S:40:LYS:HD3	2:S:40:LYS:N	2.21	0.53
2:D:65:ALA:HB1	2:D:70:GLU:HB2	1.89	0.53
3:E:701:DT:H2''	3:E:702:DG:C8	2.43	0.53
2:S:27:SER:CA	2:S:45:LYS:HG2	2.38	0.53
1:C:41:ALA:HA	1:C:44:ARG:NH1	2.23	0.53
3:E:705:DA:H2''	3:E:706:DG:O5'	2.09	0.53
3:E:710:DT:C2'	3:E:711:DT:C5'	2.80	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:O	1:A:110:LEU:HD23	2.08	0.53
1:C:118:VAL:O	1:C:141:VAL:HG11	2.08	0.53
1:C:231:LEU:HD13	1:C:255:ILE:O	2.09	0.52
1:A:70:ASP:HA	1:A:98:ASN:HD22	1.74	0.52
1:C:288:LEU:HA	1:C:331:SER:HB3	1.90	0.52
2:D:14:ILE:O	2:D:14:ILE:HG22	2.10	0.52
1:A:65:GLY:O	1:A:121:ILE:HG23	2.10	0.52
1:C:223:THR:HG22	1:C:225:ASP:N	2.25	0.52
1:A:288:LEU:O	1:A:329:ARG:HG3	2.10	0.52
2:S:7:LYS:HE3	2:S:88:GLU:HB2	1.90	0.52
2:D:8:VAL:HG23	2:D:58:GLY:N	2.24	0.52
4:B:705:DA:H2''	4:B:706:DG:O5'	2.09	0.52
1:A:128:ILE:HG22	1:A:128:ILE:O	2.09	0.52
3:E:712:DT:C2'	3:E:713:DC:H5''	2.31	0.52
1:A:31:LYS:HE2	1:A:33:THR:OG1	2.10	0.51
3:E:711:DT:H2''	3:E:712:DT:O5'	2.09	0.51
1:A:228:LEU:HA	1:A:258:ALA:HB2	1.92	0.51
1:A:257:HIS:HE1	1:C:283:MET:O	1.93	0.51
1:A:275:PHE:O	1:A:276:ASP:CB	2.58	0.51
2:D:37:TYR:HE2	2:D:59:ALA:HB1	1.75	0.51
1:A:68:ILE:CD1	1:A:76:TYR:HB3	2.41	0.51
2:D:35:LEU:O	2:D:41:THR:HA	2.10	0.51
1:A:101:GLN:HE22	1:A:126:GLY:H	1.57	0.51
2:S:14:ILE:HD13	2:S:86:LEU:HD22	1.91	0.51
2:D:53:LEU:HD23	2:D:55:ILE:HD11	1.91	0.51
2:D:8:VAL:HG23	2:D:58:GLY:H	1.76	0.51
1:A:163:GLU:OE2	1:A:200:GLY:HA2	2.11	0.51
2:S:17:ARG:O	2:S:20:THR:HB	2.11	0.51
2:D:77:LEU:O	2:D:81:MET:HB2	2.11	0.51
1:C:231:LEU:HD11	1:C:259:ALA:HB2	1.91	0.51
1:A:63:THR:CG2	1:C:116:LYS:NZ	2.72	0.50
1:A:329:ARG:HG3	1:A:329:ARG:HH11	1.77	0.50
1:A:69:PRO:HD3	1:A:124:MET:O	2.12	0.50
1:C:187:PRO:HD2	1:C:222:TYR:CZ	2.47	0.50
4:B:704:DA:H2''	4:B:705:DA:OP2	2.10	0.50
1:A:188:MET:CE	1:A:198:LEU:HD22	2.42	0.50
1:C:16:SER:HB3	4:B:702:DG:H2'	1.94	0.50
1:A:188:MET:HE1	1:A:198:LEU:HD22	1.94	0.50
1:A:71:ILE:HG12	1:A:71:ILE:O	2.12	0.50
1:C:96:LEU:HD13	1:C:97:SER:N	2.27	0.50
1:C:180:ASP:HB3	1:C:216:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ALA:HB2	2:D:44:LEU:HD12	1.94	0.50
2:S:19:ALA:O	2:S:23:VAL:HG23	2.11	0.49
2:S:23:VAL:HG13	2:S:44:LEU:O	2.12	0.49
2:D:25:THR:HA	2:D:28:LYS:HD2	1.92	0.49
3:E:714:DA:H61	4:B:701:DT:H3	1.60	0.49
1:C:68:ILE:CD1	1:C:76:TYR:HB3	2.41	0.49
1:A:79:LEU:HD13	1:A:124:MET:SD	2.51	0.49
1:C:4:ILE:HD11	1:C:46:GLY:O	2.12	0.49
1:C:269:ASP:C	1:C:270:LEU:HD12	2.33	0.49
3:E:709:DC:H2''	3:E:710:DT:O5'	2.12	0.49
1:A:328:LEU:HD12	1:A:328:LEU:N	2.22	0.49
1:C:231:LEU:CD1	1:C:259:ALA:HB2	2.42	0.49
1:C:70:ASP:HA	1:C:98:ASN:ND2	2.20	0.49
2:S:8:VAL:HG23	2:S:59:ALA:H	1.77	0.48
1:C:133:VAL:HG21	1:C:152:GLN:CG	2.35	0.48
2:D:8:VAL:HG23	2:D:8:VAL:O	2.12	0.48
1:A:256:ILE:CD1	1:A:272:ILE:HG21	2.39	0.48
1:A:10:ALA:HB1	1:A:15:VAL:O	2.13	0.48
1:A:111:ASN:O	1:A:112:THR:C	2.51	0.48
1:C:87:ALA:HB2	1:C:303:MET:CE	2.43	0.48
1:C:101:GLN:NE2	1:C:126:GLY:H	2.03	0.48
1:C:240:LYS:NZ	1:C:240:LYS:HB3	2.28	0.48
1:A:87:ALA:HB2	1:A:303:MET:HE2	1.93	0.48
1:A:192:ILE:O	1:A:196:LYS:HB2	2.13	0.48
2:S:65:ALA:O	2:S:70:GLU:HB2	2.14	0.48
1:A:50:ASN:ND2	1:C:117:GLN:OE1	2.46	0.48
1:C:272:ILE:HD12	1:C:272:ILE:N	2.29	0.48
1:C:194:ARG:O	1:C:198:LEU:HB3	2.14	0.48
1:A:94:ILE:HD11	1:A:303:MET:CE	2.42	0.48
2:S:22:LEU:HD13	2:S:81:MET:HE3	1.95	0.48
1:C:287:GLN:O	1:C:329:ARG:HB2	2.14	0.48
2:S:37:TYR:O	2:S:39:GLY:N	2.46	0.47
2:D:4:LYS:HB2	2:D:4:LYS:NZ	2.28	0.47
2:D:26:ALA:HB3	2:D:44:LEU:HD12	1.96	0.47
2:D:81:MET:HA	2:D:81:MET:CE	2.44	0.47
4:B:700:DC:H2'	4:B:701:DT:H71	1.96	0.47
1:A:34:THR:O	1:A:38:VAL:HG12	2.14	0.47
2:S:47:ILE:HG12	6:S:138:HOH:O	2.13	0.47
1:C:109:LEU:O	1:C:113:MET:HG2	2.14	0.47
1:C:166:ILE:HG13	1:C:197:LYS:HA	1.97	0.47
1:A:266:ILE:HG23	1:A:267:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD1	1:A:333:LYS:HG3	2.13	0.47
1:A:298:ILE:HD13	1:A:322:LEU:HD12	1.97	0.47
1:A:53:ALA:HB3	4:B:709:DC:H5'	1.97	0.47
2:D:37:TYR:HB2	2:D:61:ILE:HG22	1.95	0.47
3:E:712:DT:O2	4:B:703:DA:N1	2.48	0.47
1:A:228:LEU:HD12	1:A:254:GLY:O	2.14	0.47
1:A:310:MET:C	1:A:312:LYS:H	2.18	0.47
1:A:290:THR:HG22	1:A:291:VAL:O	2.15	0.47
1:C:11:ARG:C	1:C:13:ALA:H	2.17	0.47
1:C:184:VAL:HG21	1:C:255:ILE:HD11	1.97	0.47
1:A:223:THR:HG22	1:A:226:SER:H	1.79	0.46
2:S:22:LEU:CD1	2:S:81:MET:HE3	2.44	0.46
1:A:290:THR:CG2	1:A:291:VAL:N	2.77	0.46
2:S:55:ILE:HD13	2:S:61:ILE:HG21	1.96	0.46
1:C:247:ALA:O	1:C:275:PHE:HB3	2.16	0.46
1:C:68:ILE:O	1:C:98:ASN:HA	2.15	0.46
1:C:274:GLY:C	1:C:290:THR:HG23	2.35	0.46
1:A:271:ASP:O	1:A:272:ILE:HD12	2.15	0.46
1:C:101:GLN:HE22	1:C:126:GLY:N	2.03	0.46
2:D:10:ALA:HB2	2:D:86:LEU:HD23	1.96	0.46
1:A:101:GLN:NE2	1:A:126:GLY:H	2.14	0.46
1:C:286:PRO:HB2	1:C:330:LYS:O	2.16	0.46
1:C:23:VAL:HG21	1:C:38:VAL:CG1	2.44	0.46
4:B:706:DG:H4'	4:B:706:DG:OP1	2.16	0.46
2:S:70:GLU:HG3	2:S:71:ASN:N	2.30	0.46
1:C:222:TYR:HA	1:C:251:MET:HG3	1.98	0.46
2:D:5:THR:HA	2:D:61:ILE:O	2.16	0.46
2:S:2:ALA:O	2:S:3:GLN:HB2	2.16	0.45
2:S:53:LEU:HD12	2:S:53:LEU:HA	1.77	0.45
1:A:287:GLN:HB2	1:A:329:ARG:HB3	1.98	0.45
2:S:3:GLN:HG3	2:S:4:LYS:N	2.31	0.45
1:C:123:PHE:HB3	1:C:145:LEU:HD23	1.96	0.45
1:C:192:ILE:O	1:C:197:LYS:HG3	2.17	0.45
1:C:277:ASN:CG	1:C:277:ASN:O	2.55	0.45
1:A:61:THR:O	1:C:116:LYS:NZ	2.50	0.45
2:S:7:LYS:HE3	2:S:88:GLU:OE2	2.17	0.45
1:C:228:LEU:HA	1:C:258:ALA:HB2	1.98	0.45
2:D:65:ALA:HB1	2:D:70:GLU:CB	2.45	0.45
1:A:170:VAL:HG11	1:A:204:ALA:HB3	1.99	0.45
1:A:231:LEU:HD22	1:A:259:ALA:N	2.31	0.45
1:A:234:LEU:C	1:A:236:SER:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:MET:HA	1:A:235:MET:HE2	1.99	0.45
1:A:278:THR:O	1:A:279:ARG:C	2.54	0.45
2:S:35:LEU:HD11	2:S:61:ILE:HB	1.99	0.45
1:C:223:THR:O	1:C:224:TYR:C	2.53	0.45
2:S:71:ASN:O	2:S:75:ASN:HB2	2.17	0.45
1:C:284:VAL:HG12	1:C:285:ARG:N	2.31	0.45
2:D:8:VAL:HG22	2:D:59:ALA:N	2.28	0.45
3:E:711:DT:O2	4:B:704:DA:C2	2.69	0.45
1:A:22:ARG:HB3	1:A:27:ASN:HB3	1.99	0.45
1:A:221:ASP:C	1:A:223:THR:H	2.19	0.45
2:S:8:VAL:HG12	2:S:14:ILE:HD11	1.99	0.45
1:C:304:ARG:HG3	2:D:48:MET:HG3	1.99	0.45
1:A:74:ILE:HD13	1:A:74:ILE:O	2.16	0.45
1:A:174:VAL:C	1:A:176:LYS:H	2.21	0.45
1:A:306:LEU:O	1:A:310:MET:HG3	2.16	0.45
1:C:275:PHE:CD2	1:C:291:VAL:HB	2.52	0.45
1:C:245:LEU:HD12	1:C:273:ILE:O	2.17	0.44
1:A:277:ASN:ND2	1:A:292:VAL:HG22	2.32	0.44
1:A:296:TYR:C	1:A:296:TYR:CD2	2.90	0.44
2:S:29:TYR:CE2	2:S:73:ALA:HA	2.53	0.44
1:C:172:LEU:HD23	1:C:172:LEU:O	2.18	0.44
1:A:284:VAL:HG12	1:A:285:ARG:H	1.82	0.44
1:A:27:ASN:OD1	1:A:28:PRO:HD2	2.17	0.44
1:C:187:PRO:HD3	1:C:221:ASP:HA	1.99	0.44
2:S:4:LYS:HG2	2:S:6:PHE:CE1	2.52	0.44
1:C:221:ASP:OD1	1:C:226:SER:HB3	2.18	0.44
1:A:99:SER:HB2	1:A:106:GLU:HG2	2.00	0.44
2:S:43:ASN:OD1	2:S:45:LYS:HB2	2.17	0.44
1:A:326:ILE:HG22	1:A:327:GLU:N	2.33	0.43
1:C:294:PRO:HB2	1:C:297:ASP:HB2	1.98	0.43
1:A:194:ARG:HG3	1:A:195:SER:N	2.33	0.43
1:C:38:VAL:O	1:C:41:ALA:N	2.51	0.43
1:A:71:ILE:CG1	1:C:71:ILE:HD11	2.49	0.43
1:A:86:ILE:HG13	1:A:300:ALA:HB1	2.00	0.43
1:A:285:ARG:NH2	1:C:224:TYR:OH	2.51	0.43
2:S:22:LEU:HD22	2:S:81:MET:CE	2.48	0.43
1:A:221:ASP:OD1	1:A:223:THR:HB	2.18	0.43
1:C:266:ILE:HD12	1:C:272:ILE:CD1	2.48	0.43
2:D:8:VAL:CG2	2:D:59:ALA:H	2.28	0.43
1:A:54:ARG:HD3	4:B:710:DT:H5'	2.01	0.43
1:C:36:LYS:O	1:C:40:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ALA:HA	1:C:271:ASP:O	2.18	0.43
1:C:286:PRO:HB2	1:C:330:LYS:HB2	2.00	0.43
2:D:3:GLN:HE21	2:D:3:GLN:HB3	1.52	0.43
1:A:228:LEU:O	1:A:232:GLN:HG3	2.19	0.43
1:A:149:VAL:HA	6:A:344:HOH:O	2.19	0.43
1:C:150:GLU:HG2	1:C:152:GLN:HE21	1.84	0.43
1:A:71:ILE:HG22	1:A:98:ASN:HD21	1.84	0.43
1:A:216:PHE:CD2	1:A:241:PRO:HG3	2.53	0.43
1:C:275:PHE:HD2	1:C:291:VAL:HG21	1.83	0.43
3:E:704:DT:C2'	3:E:705:DA:H5'	2.48	0.43
1:A:231:LEU:HD22	1:A:258:ALA:CB	2.48	0.42
2:S:22:LEU:HD22	2:S:81:MET:HE1	2.01	0.42
1:C:54:ARG:HD3	6:C:352:HOH:O	2.18	0.42
1:A:89:MET:HG3	2:S:24:GLN:HE21	1.84	0.42
1:A:151:GLU:O	1:A:153:GLU:HG2	2.19	0.42
1:A:178:HIS:CE1	1:A:243:ALA:HB2	2.54	0.42
1:C:193:ASN:HD22	1:C:193:ASN:HA	1.71	0.42
1:C:18:ALA:HB2	4:B:703:DA:H62	1.84	0.42
1:A:71:ILE:H	1:A:98:ASN:HD21	1.64	0.42
1:A:224:TYR:HB2	1:C:283:MET:CE	2.49	0.42
1:C:276:ASP:H	1:C:290:THR:CG2	2.33	0.42
1:C:275:PHE:O	1:C:276:ASP:CB	2.67	0.42
1:A:151:GLU:N	1:A:152:GLN:HE21	2.17	0.42
1:A:276:ASP:O	1:A:277:ASN:HB3	2.20	0.42
2:S:27:SER:HA	2:S:45:LYS:CG	2.45	0.42
2:D:69:ASP:C	2:D:71:ASN:H	2.23	0.42
2:S:38:ASN:OD1	2:S:38:ASN:O	2.37	0.42
2:S:81:MET:HA	2:S:81:MET:HE2	2.01	0.42
2:S:81:MET:HE2	2:S:86:LEU:HD12	2.02	0.42
1:A:221:ASP:OD1	1:A:223:THR:HG22	2.20	0.41
1:A:266:ILE:N	1:A:266:ILE:HD12	2.35	0.41
1:C:278:THR:C	1:C:280:LEU:N	2.74	0.41
2:S:2:ALA:HB1	2:S:74:LEU:HD13	2.02	0.41
1:C:240:LYS:HA	1:C:241:PRO:HD3	1.93	0.41
1:C:249:ASP:O	1:C:253:LEU:HD13	2.20	0.41
1:C:320:VAL:HG12	1:C:321:GLU:N	2.35	0.41
2:D:14:ILE:CD1	2:D:86:LEU:HD22	2.50	0.41
1:A:103:MET:HE1	1:A:129:THR:HG21	2.02	0.41
1:A:231:LEU:HD22	1:A:258:ALA:C	2.40	0.41
1:C:172:LEU:O	1:C:176:LYS:HG3	2.20	0.41
1:C:195:SER:O	1:C:196:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HG2	1:A:33:THR:H	1.86	0.41
1:C:307:THR:HA	1:C:310:MET:CE	2.50	0.41
2:D:12:SER:O	2:D:15:HIS:HD2	2.04	0.41
1:A:116:LYS:HE3	1:C:63:THR:OG1	2.20	0.41
1:C:27:ASN:HA	1:C:28:PRO:HD3	1.95	0.41
2:D:46:SEP:O2P	2:D:48:MET:HB2	2.20	0.41
1:A:251:MET:HB2	1:A:251:MET:HE2	1.96	0.41
1:C:209:ASN:HD22	1:C:209:ASN:HA	1.64	0.41
1:C:311:ASN:HB3	1:C:313:GLU:HG2	2.03	0.41
1:A:38:VAL:O	1:A:42:ILE:HG13	2.21	0.41
1:A:216:PHE:CE2	1:A:241:PRO:HG3	2.55	0.41
2:S:8:VAL:HG23	2:S:58:GLY:N	2.29	0.41
2:S:9:THR:HG23	2:S:87:GLY:HA2	2.02	0.41
1:C:198:LEU:O	1:C:201:TYR:HB3	2.20	0.41
1:A:6:ILE:HG13	1:A:20:VAL:CG1	2.50	0.41
1:A:64:VAL:HG21	1:A:303:MET:HE3	2.03	0.41
1:A:113:MET:C	1:A:115:GLY:N	2.74	0.41
1:A:215:GLN:HB3	1:A:237:LEU:CD1	2.51	0.41
1:C:10:ALA:HB1	1:C:15:VAL:O	2.21	0.41
1:C:15:VAL:HB	1:C:19:THR:OG1	2.21	0.41
1:C:33:THR:O	1:C:37:LYS:HB2	2.20	0.41
1:C:253:LEU:N	1:C:253:LEU:HD12	2.36	0.41
1:C:296:TYR:CD2	2:D:16:ALA:HA	2.56	0.41
3:E:703:DT:N3	4:B:712:DA:H2	2.02	0.41
1:A:31:LYS:HB3	1:A:34:THR:OG1	2.21	0.40
1:A:118:VAL:O	1:A:141:VAL:HG11	2.21	0.40
1:C:163:GLU:O	1:C:200:GLY:HA3	2.22	0.40
1:C:192:ILE:O	1:C:192:ILE:HG13	2.20	0.40
1:C:280:LEU:C	1:C:282:LEU:H	2.24	0.40
2:D:4:LYS:O	2:D:62:THR:HA	2.22	0.40
2:D:17:ARG:HB2	2:D:18:PRO:HD3	2.02	0.40
2:D:22:LEU:HD13	2:D:81:MET:HE3	2.04	0.40
2:D:27:SER:HB3	2:D:45:LYS:HB3	2.03	0.40
1:A:162:TYR:CE2	1:A:192:ILE:HD11	2.57	0.40
1:A:131:GLU:O	1:A:134:ALA:HB3	2.20	0.40
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.84	0.40
1:C:19:THR:HG23	1:C:22:ARG:HH11	1.85	0.40
1:A:54:ARG:HD3	4:B:710:DT:C5'	2.52	0.40
1:A:68:ILE:CG1	1:A:124:MET:HE3	2.44	0.40
1:A:158:VAL:HG21	1:A:302:ALA:HA	2.04	0.40
1:C:39:LEU:O	1:C:42:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	331/339 (98%)	281 (85%)	43 (13%)	7 (2%)	5	25
1	C	330/339 (97%)	279 (84%)	43 (13%)	8 (2%)	5	22
2	D	84/87 (97%)	64 (76%)	13 (16%)	7 (8%)	0	3
2	S	84/87 (97%)	70 (83%)	11 (13%)	3 (4%)	3	14
All	All	829/852 (97%)	694 (84%)	110 (13%)	25 (3%)	3	17

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	29	ASN
1	A	276	ASP
2	S	38	ASN
1	C	276	ASP
2	D	65	ALA
2	D	69	ASP
1	A	175	ASP
1	C	12	GLU
2	D	55	ILE
2	S	4	LYS
1	C	3	ASN
1	C	236	SER
2	D	64	SER
2	S	68	ALA
1	C	29	ASN
1	C	317	GLU
1	A	30	VAL
1	A	317	GLU
2	D	68	ALA

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Mol	Chain	Res	Type
2	D	70	GLU
2	D	79	GLU
1	A	256	ILE
1	C	158	VAL
1	C	239	LYS

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	286/292 (98%)	266 (93%)	20 (7%)	12	39
1	C	286/292 (98%)	263 (92%)	23 (8%)	10	33
2	D	66/66 (100%)	59 (89%)	7 (11%)	5	21
2	S	66/66 (100%)	56 (85%)	10 (15%)	2	10
All	All	704/716 (98%)	644 (92%)	60 (8%)	8	31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	30	VAL
1	A	48	ARG
1	A	54	ARG
1	A	56	LEU
1	A	60	LYS
1	A	74	ILE
1	A	79	LEU
1	A	81	ARG
1	A	96	LEU
1	A	97	SER
1	A	105	LYS
1	A	151	GLU
1	A	152	GLN
1	A	223	THR
1	A	231	LEU

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	309	LEU
1	A	316	GLU
1	A	328	LEU
2	S	3	GLN
2	S	9	THR
2	S	11	ASP
2	S	17	ARG
2	S	27	SER
2	S	40	LYS
2	S	44	LEU
2	S	53	LEU
2	S	72	ASP
2	S	74	LEU
1	C	11	ARG
1	C	48	ARG
1	C	56	LEU
1	C	61	THR
1	C	62	THR
1	C	79	LEU
1	C	86	ILE
1	C	93	ASN
1	C	94	ILE
1	C	96	LEU
1	C	101	GLN
1	C	110	LEU
1	C	111	ASN
1	C	152	GLN
1	C	164	GLN
1	C	237	LEU
1	C	240	LYS
1	C	264	LEU
1	C	271	ASP
1	C	285	ARG
1	C	312	LYS
1	C	325	ARG
1	C	328	LEU
2	D	3	GLN
2	D	4	LYS
2	D	17	ARG
2	D	36	GLU
2	D	44	LEU

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Mol	Chain	Res	Type
2	D	81	MET
2	D	84	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	152	GLN
1	A	215	GLN
1	A	232	GLN
1	A	262	GLN
1	A	277	ASN
1	A	293	GLN
1	A	311	ASN
2	S	3	GLN
2	S	24	GLN
1	C	98	ASN
1	C	101	GLN
1	C	102	ASN
1	C	152	GLN
1	C	209	ASN
1	C	232	GLN
1	C	262	GLN
1	C	293	GLN
1	C	311	ASN
2	D	3	GLN
2	D	15	HIS
2	D	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	D	46	2	8,9,10	0.96	0	7,12,14	1.81	2 (28%)
2	SEP	S	46	2	8,9,10	1.00	1 (12%)	7,12,14	1.45	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	D	46	2	-	6/6/8/10	-
2	SEP	S	46	2	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	46	SEP	P-O3P	-2.08	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	46	SEP	OG-CB-CA	3.28	111.34	108.14
2	D	46	SEP	O3P-P-O1P	2.73	121.48	110.83
2	S	46	SEP	OG-CB-CA	2.39	110.47	108.14
2	S	46	SEP	O3P-P-O1P	2.33	119.92	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	46	SEP	C-CA-CB-OG
2	S	46	SEP	CB-OG-P-O1P
2	S	46	SEP	CB-OG-P-O2P
2	S	46	SEP	CB-OG-P-O3P
2	D	46	SEP	N-CA-CB-OG
2	D	46	SEP	C-CA-CB-OG
2	D	46	SEP	CA-CB-OG-P

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Mol	Chain	Res	Type	Atoms
2	D	46	SEP	CB-OG-P-O2P
2	D	46	SEP	CB-OG-P-O3P
2	S	46	SEP	CA-CB-OG-P
2	S	46	SEP	N-CA-CB-OG
2	D	46	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	46	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	$\# Z > 2$
5	SO4	C	699	-	4,4,4	0.37	0	6,6,6	0.10	0
5	SO4	C	599	-	4,4,4	0.37	0	6,6,6	0.10	0
5	SO4	C	999	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	A	399	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	A	499	-	4,4,4	0.41	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/339 (98%)	-0.44	1 (0%) 90 83	48, 74, 107, 142	0
1	C	332/339 (97%)	-0.35	1 (0%) 90 83	46, 87, 124, 142	0
2	D	86/87 (98%)	0.18	2 (2%) 61 44	71, 116, 132, 142	0
2	S	86/87 (98%)	-0.40	0 100 100	58, 89, 111, 124	0
3	E	16/16 (100%)	-0.15	0 100 100	66, 81, 98, 100	0
4	B	16/16 (100%)	-0.19	0 100 100	66, 79, 98, 99	0
All	All	869/884 (98%)	-0.33	4 (0%) 87 77	46, 83, 123, 142	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	6.4
1	C	151	GLU	2.3
2	D	17	ARG	2.2
2	D	64	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	D	46	10/11	0.94	0.07	88,93,97,99	0
2	SEP	S	46	10/11	0.99	0.03	51,62,65,71	0

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(\AA^2)	Q<0.9
5	SO4	C	699	5/5	0.71	0.09	165,166,167,168	0
5	SO4	C	599	5/5	0.76	0.12	152,152,154,155	0
5	SO4	C	999	5/5	0.79	0.11	177,178,178,178	0
5	SO4	A	399	5/5	0.82	0.10	131,135,138,138	0
5	SO4	A	499	5/5	0.84	0.12	126,127,132,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.