



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 02:37 PM EDT

PDB ID : 9OTL / pdb_00009otl
Title : Crystal Structure of Salmonella FraB Deglycase, Crystal Form 1
Authors : Bell, C.E.; Zakharova, K.
Deposited on : 2025-05-27
Resolution : 1.85 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 : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

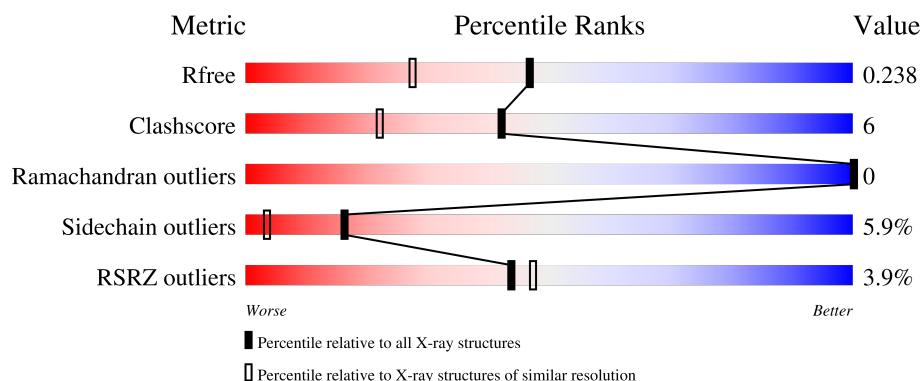
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	345	<div> <div>9%</div> <div>78%</div> <div>11%</div> <div>8%</div> </div>
1	B	345	<div> <div>80%</div> <div>12%</div> <div>6%</div> </div>
1	C	345	<div> <div>9%</div> <div>68%</div> <div>22%</div> <div>8%</div> </div>
1	D	345	<div> <div>3%</div> <div>73%</div> <div>14%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10398 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 SIS domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2480	1589	418	461	12			
1	B	324	Total	C	N	O	S	0	0	0
			2526	1617	424	474	11			
1	C	319	Total	C	N	O	S	0	0	0
			2475	1583	411	469	12			
1	D	310	Total	C	N	O	S	0	0	0
			2385	1525	398	452	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP V7IWJ0
A	-18	ASP	-	expression tag	UNP V7IWJ0
A	-17	HIS	-	expression tag	UNP V7IWJ0
A	-16	HIS	-	expression tag	UNP V7IWJ0
A	-15	HIS	-	expression tag	UNP V7IWJ0
A	-14	HIS	-	expression tag	UNP V7IWJ0
A	-13	HIS	-	expression tag	UNP V7IWJ0
A	-12	HIS	-	expression tag	UNP V7IWJ0
A	-11	GLU	-	expression tag	UNP V7IWJ0
A	-10	ASN	-	expression tag	UNP V7IWJ0
A	-9	LEU	-	expression tag	UNP V7IWJ0
A	-8	TYR	-	expression tag	UNP V7IWJ0
A	-7	PHE	-	expression tag	UNP V7IWJ0
A	-6	GLN	-	expression tag	UNP V7IWJ0
A	275	ALA	LYS	engineered mutation	UNP V7IWJ0
A	276	ALA	GLU	engineered mutation	UNP V7IWJ0
B	-19	MET	-	expression tag	UNP V7IWJ0
B	-18	ASP	-	expression tag	UNP V7IWJ0
B	-17	HIS	-	expression tag	UNP V7IWJ0
B	-16	HIS	-	expression tag	UNP V7IWJ0
B	-15	HIS	-	expression tag	UNP V7IWJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP V7IWJ0
B	-13	HIS	-	expression tag	UNP V7IWJ0
B	-12	HIS	-	expression tag	UNP V7IWJ0
B	-11	GLU	-	expression tag	UNP V7IWJ0
B	-10	ASN	-	expression tag	UNP V7IWJ0
B	-9	LEU	-	expression tag	UNP V7IWJ0
B	-8	TYR	-	expression tag	UNP V7IWJ0
B	-7	PHE	-	expression tag	UNP V7IWJ0
B	-6	GLN	-	expression tag	UNP V7IWJ0
B	275	ALA	LYS	engineered mutation	UNP V7IWJ0
B	276	ALA	GLU	engineered mutation	UNP V7IWJ0
C	-19	MET	-	expression tag	UNP V7IWJ0
C	-18	ASP	-	expression tag	UNP V7IWJ0
C	-17	HIS	-	expression tag	UNP V7IWJ0
C	-16	HIS	-	expression tag	UNP V7IWJ0
C	-15	HIS	-	expression tag	UNP V7IWJ0
C	-14	HIS	-	expression tag	UNP V7IWJ0
C	-13	HIS	-	expression tag	UNP V7IWJ0
C	-12	HIS	-	expression tag	UNP V7IWJ0
C	-11	GLU	-	expression tag	UNP V7IWJ0
C	-10	ASN	-	expression tag	UNP V7IWJ0
C	-9	LEU	-	expression tag	UNP V7IWJ0
C	-8	TYR	-	expression tag	UNP V7IWJ0
C	-7	PHE	-	expression tag	UNP V7IWJ0
C	-6	GLN	-	expression tag	UNP V7IWJ0
C	275	ALA	LYS	engineered mutation	UNP V7IWJ0
C	276	ALA	GLU	engineered mutation	UNP V7IWJ0
D	-19	MET	-	expression tag	UNP V7IWJ0
D	-18	ASP	-	expression tag	UNP V7IWJ0
D	-17	HIS	-	expression tag	UNP V7IWJ0
D	-16	HIS	-	expression tag	UNP V7IWJ0
D	-15	HIS	-	expression tag	UNP V7IWJ0
D	-14	HIS	-	expression tag	UNP V7IWJ0
D	-13	HIS	-	expression tag	UNP V7IWJ0
D	-12	HIS	-	expression tag	UNP V7IWJ0
D	-11	GLU	-	expression tag	UNP V7IWJ0
D	-10	ASN	-	expression tag	UNP V7IWJ0
D	-9	LEU	-	expression tag	UNP V7IWJ0
D	-8	TYR	-	expression tag	UNP V7IWJ0
D	-7	PHE	-	expression tag	UNP V7IWJ0
D	-6	GLN	-	expression tag	UNP V7IWJ0
D	275	ALA	LYS	engineered mutation	UNP V7IWJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	276	ALA	GLU	engineered mutation	UNP V7IWJ0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

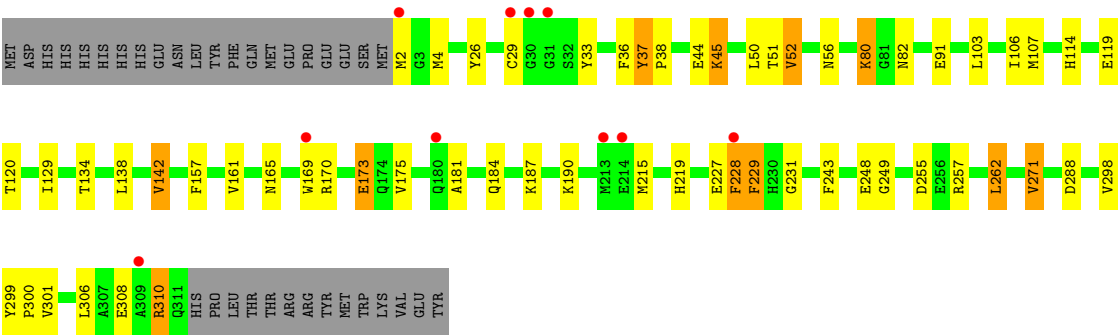
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	143	Total O 143 143	0	0
3	B	165	Total O 165 165	0	0
3	C	90	Total O 90 90	0	0
3	D	131	Total O 131 131	0	0

- Molecule 1: SIS domain protein



● Molecule 1: SIS domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.12Å 115.77Å 108.31Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	107.81 – 1.85 107.81 – 1.85	Depositor EDS
% Data completeness (in resolution range)	76.4 (107.81-1.85) 76.4 (107.81-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.186 , 0.233 0.195 , 0.238	Depositor DCC
R_{free} test set	4873 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10398	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.74	0/2540	1.25	14/3442 (0.4%)
1	B	0.73	1/2589 (0.0%)	1.26	13/3514 (0.4%)
1	C	0.64	0/2534	1.23	10/3439 (0.3%)
1	D	0.67	0/2442	1.25	11/3317 (0.3%)
All	All	0.70	1/10105 (0.0%)	1.25	48/13712 (0.4%)

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ILE	CB-CG1	-5.34	1.42	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	PHE	CA-CB-CG	-9.56	104.24	113.80
1	A	149	GLU	N-CA-CB	-9.15	98.83	111.00
1	D	82	ASN	CB-CA-C	-8.97	94.31	109.38
1	B	227	GLU	CB-CA-C	8.03	125.15	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	VAL	CB-CA-C	-7.55	98.60	110.69
1	C	216	GLN	CB-CA-C	-7.37	101.04	111.80
1	A	142	VAL	N-CA-CB	7.32	120.50	110.54
1	A	248	GLU	CB-CA-C	7.05	122.06	109.38
1	A	227	GLU	CB-CA-C	-7.00	95.33	109.55
1	D	271	VAL	N-CA-CB	6.84	119.20	110.99
1	B	316	THR	CA-CB-OG1	-6.80	99.40	109.60
1	C	319	TYR	CB-CA-C	6.71	120.82	109.75
1	C	52	VAL	CB-CA-C	-6.69	100.20	110.50
1	C	288	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	13	THR	CA-CB-OG1	-6.67	99.60	109.60
1	C	52	VAL	N-CA-CB	6.54	122.17	111.44
1	B	50	LEU	N-CA-CB	-6.45	99.97	110.81
1	A	227	GLU	N-CA-CB	6.35	120.35	110.44
1	C	128	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	50	LEU	N-CA-CB	-6.31	99.88	110.80
1	A	215	MET	CG-SD-CE	-6.25	87.14	100.90
1	D	173	GLU	CB-CG-CD	6.24	123.20	112.60
1	A	194	THR	CA-CB-OG1	-6.21	100.28	109.60
1	B	108	ASP	CB-CA-C	-6.21	97.80	109.72
1	D	142	VAL	N-CA-CB	6.19	119.87	110.58
1	D	227	GLU	CB-CA-C	6.16	122.21	109.95
1	A	288	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	108	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	228	PHE	CB-CA-C	-5.90	98.68	110.42
1	B	308	GLU	CB-CA-C	5.90	121.99	110.67
1	B	86	THR	CA-CB-OG1	-5.85	100.82	109.60
1	A	56	ASN	CB-CA-C	5.65	119.32	109.65
1	A	50	LEU	N-CA-CB	-5.61	101.29	110.43
1	D	255	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	120	THR	CA-CB-OG1	-5.46	101.42	109.60
1	C	304	ARG	CB-CA-C	5.41	119.45	110.90
1	B	288	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	138	LEU	N-CA-CB	-5.32	102.03	110.22
1	D	37	TYR	CA-C-O	5.30	123.48	118.34
1	D	37	TYR	O-C-N	-5.28	115.75	120.71
1	B	212	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	290	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	103	LEU	N-CA-CB	-5.18	102.56	110.65
1	A	44	GLU	CB-CA-C	5.18	120.62	110.67
1	A	36	PHE	CA-CB-CG	5.15	118.95	113.80
1	C	298	VAL	N-CA-CB	-5.08	100.89	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	TYR	CB-CA-C	5.06	119.19	110.79
1	B	234	GLU	CB-CG-CD	5.02	121.14	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	ARG	Sidechain
1	B	2	MET	Peptide
1	C	304	ARG	Sidechain
1	D	310	ARG	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	2480	0	2394	29	0
1	B	2526	0	2430	18	0
1	C	2475	0	2362	50	0
1	D	2385	0	2283	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
3	A	143	0	0	2	0
3	B	165	0	0	3	0
3	C	90	0	0	6	0
3	D	131	0	0	3	0
All	All	10398	0	9469	119	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 6.

All (119) 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:A:51:THR:HG22	1:B:51:THR:HG22	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:HG22	1:D:51:THR:HG22	1.52	0.89
1:A:227:GLU:HG3	3:A:607:HOH:O	1.73	0.87
1:D:44:GLU:OE2	3:D:501:HOH:O	2.07	0.73
1:B:216:GLN:HE22	1:B:319:TYR:H	1.37	0.72
1:C:167:ILE:O	3:C:401:HOH:O	2.11	0.68
1:D:170:ARG:O	1:D:173:GLU:HG3	1.94	0.68
1:C:129:ILE:H	1:C:165:ASN:HD22	1.40	0.67
1:C:227:GLU:OE1	3:C:402:HOH:O	2.11	0.67
1:C:109:SER:OG	1:C:110:PRO:HD2	1.96	0.66
1:A:112:VAL:HG13	1:A:118:VAL:HG21	1.78	0.66
1:C:197:SER:O	3:C:403:HOH:O	2.13	0.65
1:D:175:VAL:HG23	1:D:301:VAL:HG11	1.79	0.65
1:D:91:GLU:OE1	1:D:114:HIS:ND1	2.24	0.64
1:A:320:MET:HE2	1:A:320:MET:N	2.14	0.63
1:C:63:ASN:OD1	1:D:45:LYS:NZ	2.31	0.63
1:D:80:LYS:HA	1:D:106:ILE:HD12	1.80	0.63
1:A:306:LEU:HD22	1:A:310:ARG:HD3	1.82	0.62
1:C:282:ILE:O	3:C:404:HOH:O	2.16	0.62
1:C:82:ASN:N	1:C:82:ASN:OD1	2.33	0.62
1:B:306:LEU:HD22	1:B:310:ARG:HD3	1.82	0.61
1:A:166:ARG:NH2	3:A:501:HOH:O	2.33	0.61
1:C:137:GLY:O	1:C:140:SER:OG	2.14	0.60
1:C:191:VAL:O	1:C:192:ILE:HD13	2.03	0.59
1:B:23:HIS:HE1	3:B:645:HOH:O	1.84	0.59
1:D:129:ILE:H	1:D:165:ASN:HD22	1.52	0.58
1:C:109:SER:O	1:C:112:VAL:HG22	2.04	0.56
1:C:109:SER:OG	1:C:110:PRO:CD	2.54	0.56
1:A:322:LYS:O	1:B:231:GLY:HA2	2.07	0.55
1:C:187:LYS:HD3	1:C:309:ALA:O	2.07	0.55
1:C:191:VAL:C	1:C:192:ILE:HD13	2.31	0.55
1:A:91:GLU:HG2	1:A:114:HIS:ND1	2.23	0.54
1:C:299:TYR:N	1:C:300:PRO:CD	2.71	0.53
1:D:157:PHE:O	1:D:161:VAL:HG23	2.09	0.53
1:D:26:TYR:HB3	1:D:36:PHE:CD2	2.44	0.53
1:C:273:ASP:O	1:C:277:LEU:HD13	2.09	0.53
1:C:243:PHE:HE1	1:C:299:TYR:CE1	2.27	0.52
1:C:28:ALA:HB1	1:C:32:SER:HB2	1.91	0.52
1:C:91:GLU:OE1	1:C:114:HIS:HD2	1.92	0.52
1:C:91:GLU:O	1:C:95:GLN:NE2	2.43	0.52
1:A:318:ARG:HB2	1:A:320:MET:HE1	1.91	0.51
1:C:112:VAL:HG12	1:C:118:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:CG2	1:C:121:TYR:N	2.74	0.51
1:C:107:MET:O	1:C:107:MET:HG2	2.09	0.50
1:C:156:ASP:O	1:C:159:ASP:HB3	2.12	0.50
1:D:215:MET:HB2	3:D:577:HOH:O	2.11	0.50
1:C:72:ALA:O	1:C:99:PRO:HD2	2.12	0.50
1:C:126:GLY:HA2	1:C:169:TRP:CZ2	2.46	0.50
1:D:4:MET:HE1	1:D:119:GLU:HG3	1.94	0.50
1:B:306:LEU:HD22	1:B:310:ARG:CD	2.42	0.49
1:A:192:ILE:HG12	1:A:241:PRO:HG2	1.94	0.49
1:A:180:GLN:HE21	1:A:180:GLN:N	2.10	0.49
1:D:129:ILE:H	1:D:165:ASN:ND2	2.11	0.49
1:C:28:ALA:O	1:C:56:ASN:HA	2.12	0.49
1:B:279:LEU:HG	1:B:294:LEU:HD22	1.94	0.49
1:A:167:ILE:HD11	1:A:281:THR:HG22	1.93	0.49
1:A:91:GLU:HG2	1:A:114:HIS:HD1	1.77	0.48
1:C:214:GLU:HG3	1:C:215:MET:CE	2.43	0.48
1:A:229:PHE:HB2	1:A:230:HIS:CD2	2.48	0.48
1:D:243:PHE:HE1	1:D:299:TYR:CE1	2.31	0.48
1:B:180:GLN:NE2	3:B:502:HOH:O	2.36	0.48
1:C:163:LYS:O	1:C:167:ILE:HG13	2.14	0.48
1:D:299:TYR:N	1:D:300:PRO:CD	2.77	0.48
1:D:249:GLY:HA3	1:D:288:ASP:OD1	2.14	0.47
1:C:214:GLU:HG3	1:C:215:MET:HE2	1.96	0.47
1:D:229:PHE:CE2	1:D:257:ARG:HG2	2.49	0.47
1:C:192:ILE:HD12	1:C:241:PRO:HG2	1.96	0.47
1:C:103:LEU:HD21	1:C:136:LYS:HB2	1.96	0.47
1:C:273:ASP:OD1	1:C:273:ASP:C	2.58	0.47
1:D:2:MET:N	3:D:508:HOH:O	2.48	0.46
1:A:133:LYS:NZ	1:A:325:TYR:O	2.34	0.46
1:D:33:TYR:C	1:D:33:TYR:CD1	2.94	0.46
1:A:180:GLN:NE2	1:A:180:GLN:CA	2.79	0.46
1:A:163:LYS:HD3	1:A:281:THR:HG23	1.98	0.46
1:B:2:MET:CB	1:B:5:LYS:H	2.29	0.45
1:C:30:GLY:O	1:C:33:TYR:HB3	2.16	0.45
1:C:94:ARG:HG3	3:C:435:HOH:O	2.15	0.45
1:D:165:ASN:HD21	1:D:169:TRP:HE1	1.65	0.45
1:A:79:HIS:HA	1:A:121:TYR:OH	2.17	0.45
1:C:228:PHE:O	1:C:233:PHE:HE2	1.99	0.45
1:C:192:ILE:HB	1:C:211:ILE:HG21	1.97	0.45
1:D:37:TYR:N	1:D:38:PRO:CD	2.80	0.45
1:D:103:LEU:HD12	1:D:119:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:O	1:A:215:MET:HB3	2.17	0.44
1:A:318:ARG:O	1:A:320:MET:HE1	2.16	0.44
1:C:215:MET:HE3	1:C:306:LEU:HD21	1.98	0.44
1:A:306:LEU:HD22	1:A:310:ARG:CD	2.46	0.44
1:B:239:ASN:HD22	1:B:267:ARG:HH12	1.65	0.44
1:D:187:LYS:HA	1:D:310:ARG:HD2	1.99	0.44
1:D:181:ALA:O	1:D:184:GLN:N	2.51	0.44
1:A:319:TYR:C	1:A:320:MET:HE2	2.43	0.44
1:B:230:HIS:HB2	3:B:635:HOH:O	2.18	0.44
1:A:37:TYR:HB3	1:A:38:PRO:HD3	2.00	0.43
1:C:42:PHE:HA	1:C:289:TYR:CE1	2.53	0.43
1:C:120:THR:HG22	1:C:121:TYR:N	2.34	0.43
1:B:185:GLU:HG2	1:B:186:TYR:CE2	2.53	0.43
1:C:234:GLU:OE2	1:D:219:HIS:ND1	2.41	0.43
1:B:37:TYR:N	1:B:38:PRO:CD	2.82	0.43
1:C:322:LYS:O	1:D:231:GLY:HA2	2.18	0.43
1:A:249:GLY:HA3	1:A:288:ASP:OD1	2.19	0.43
1:C:23:HIS:HD2	1:C:51:THR:OG1	2.02	0.42
1:A:232:PRO:CG	1:B:209:ILE:HD13	2.50	0.42
1:C:177:GLU:HB2	3:C:458:HOH:O	2.18	0.42
1:A:180:GLN:N	1:A:180:GLN:NE2	2.67	0.42
1:A:318:ARG:C	1:A:320:MET:HE1	2.45	0.42
1:C:31:GLY:HA2	1:C:206:LEU:HD21	2.03	0.41
1:C:239:ASN:O	1:C:239:ASN:CG	2.64	0.41
1:C:268:ARG:C	1:C:269:ILE:HG13	2.45	0.41
1:C:175:VAL:HG23	1:C:301:VAL:HG11	2.02	0.41
1:B:21:VAL:HG13	1:B:73:VAL:HG23	2.02	0.41
1:A:40:LYS:HE3	1:A:44:GLU:OE2	2.20	0.41
1:D:4:MET:CE	1:D:119:GLU:HG3	2.50	0.41
1:D:190:LYS:O	1:D:215:MET:HB3	2.21	0.41
1:B:79:HIS:HA	1:B:121:TYR:OH	2.20	0.41
1:B:175:VAL:HG23	1:B:301:VAL:HG11	2.03	0.41
1:B:178:ARG:HA	1:B:178:ARG:HD2	1.89	0.41
1:C:165:ASN:HD21	1:C:169:TRP:HE1	1.69	0.41
1:A:28:ALA:O	1:A:56:ASN:HA	2.21	0.40
1:D:228:PHE:CZ	1:D:262:LEU:HD11	2.56	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	314/345 (91%)	309 (98%)	5 (2%)	0	100	100
1	B	322/345 (93%)	319 (99%)	3 (1%)	0	100	100
1	C	315/345 (91%)	303 (96%)	12 (4%)	0	100	100
1	D	308/345 (89%)	303 (98%)	5 (2%)	0	100	100
All	All	1259/1380 (91%)	1234 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	251/282 (89%)	237 (94%)	14 (6%)	17	3
1	B	257/282 (91%)	244 (95%)	13 (5%)	20	5
1	C	250/282 (89%)	235 (94%)	15 (6%)	16	3
1	D	241/282 (86%)	224 (93%)	17 (7%)	12	2
All	All	999/1128 (89%)	940 (94%)	59 (6%)	16	3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	40	LYS

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Mol	Chain	Res	Type
1	A	56	ASN
1	A	88	LYS
1	A	138	LEU
1	A	142	VAL
1	A	166	ARG
1	A	178	ARG
1	A	180	GLN
1	A	185	GLU
1	A	281	THR
1	A	306	LEU
1	A	320	MET
1	A	322	LYS
1	B	29	CYS
1	B	56	ASN
1	B	88	LYS
1	B	138	LEU
1	B	208	SER
1	B	209	ILE
1	B	262	LEU
1	B	279	LEU
1	B	284	THR
1	B	306	LEU
1	B	308	GLU
1	B	322	LYS
1	B	324	GLU
1	C	9	SER
1	C	15	GLN
1	C	52	VAL
1	C	66	VAL
1	C	75	VAL
1	C	94	ARG
1	C	95	GLN
1	C	103	LEU
1	C	120	THR
1	C	125	ASP
1	C	142	VAL
1	C	264	LYS
1	C	268	ARG
1	C	283	LYS
1	C	320	MET
1	D	29	CYS
1	D	45	LYS

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Mol	Chain	Res	Type
1	D	52	VAL
1	D	56	ASN
1	D	80	LYS
1	D	107	MET
1	D	134	THR
1	D	138	LEU
1	D	142	VAL
1	D	228	PHE
1	D	229	PHE
1	D	248	GLU
1	D	262	LEU
1	D	271	VAL
1	D	298	VAL
1	D	306	LEU
1	D	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLN
1	A	23	HIS
1	A	95	GLN
1	A	180	GLN
1	A	224	HIS
1	B	10	ASN
1	B	15	GLN
1	B	23	HIS
1	B	95	GLN
1	B	153	HIS
1	B	216	GLN
1	B	224	HIS
1	B	239	ASN
1	B	245	GLN
1	C	10	ASN
1	C	23	HIS
1	C	114	HIS
1	C	146	GLN
1	C	165	ASN
1	D	79	HIS
1	D	153	HIS
1	D	165	ASN

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Mol	Chain	Res	Type
1	D	245	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	318/345 (92%)	-0.06	3 (0%) 81 87	17, 28, 44, 58	0
1	B	324/345 (93%)	0.03	5 (1%) 71 79	18, 29, 50, 76	0
1	C	319/345 (92%)	0.94	31 (9%) 15 15	25, 43, 70, 91	0
1	D	310/345 (89%)	0.30	10 (3%) 50 54	20, 35, 60, 76	0
All	All	1271/1380 (92%)	0.30	49 (3%) 44 47	17, 33, 60, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	PHE	5.1
1	A	229	PHE	4.9
1	C	316	THR	4.5
1	D	169	TRP	4.2
1	B	2	MET	4.1
1	C	107	MET	4.0
1	C	233	PHE	3.9
1	C	106	ILE	3.6
1	B	325	TYR	3.6
1	C	105	TRP	3.3
1	D	228	PHE	3.3
1	C	323	VAL	3.2
1	C	325	TYR	3.2
1	C	117	TYR	3.1
1	C	2	MET	3.0
1	C	123	PHE	3.0
1	C	176	ALA	2.9
1	C	87	ILE	2.8
1	C	169	TRP	2.8
1	C	12	VAL	2.8
1	B	108	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	2.7
1	C	29	CYS	2.6
1	C	118	VAL	2.6
1	C	126	GLY	2.6
1	C	109	SER	2.6
1	D	31	GLY	2.6
1	C	235	ILE	2.6
1	C	308	GLU	2.5
1	C	231	GLY	2.5
1	B	169	TRP	2.5
1	A	230	HIS	2.4
1	C	167	ILE	2.3
1	D	29	CYS	2.3
1	C	10	ASN	2.2
1	C	3	GLY	2.2
1	D	30	GLY	2.2
1	D	214	GLU	2.2
1	D	2	MET	2.2
1	C	317	ARG	2.2
1	C	101	ILE	2.1
1	C	318	ARG	2.1
1	D	309	ALA	2.1
1	C	309	ALA	2.1
1	C	79	HIS	2.0
1	D	180	GLN	2.0
1	C	205	TYR	2.0
1	D	213	MET	2.0
1	A	228	PHE	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 oligosaccharides 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
2	MG	D	401	1/1	0.95	0.06	46,46,46,46	0
2	MG	A	401	1/1	0.96	0.11	36,36,36,36	0
2	MG	B	401	1/1	0.98	0.09	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.