



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 2DSO / pdb_00002dso
Title : Crystal structure of D138N mutant of Drp35, a 35kDa drug responsive protein from *Staphylococcus aureus*
Authors : Tanaka, Y.; Ohki, Y.; Morikawa, K.; Yao, M.; Watanabe, N.; Ohta, T.; Tanaka, I.
Deposited on : 2006-07-04
Resolution : 2.10 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

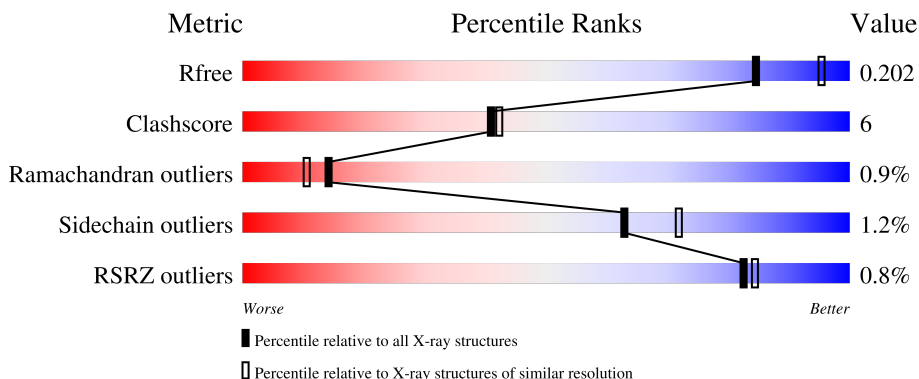
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



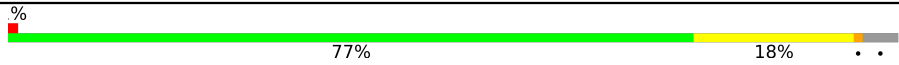
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	333	 81% 15% 2% 2%
1	B	333	 79% 16% 2% 2%
1	C	333	 74% 22% 2% 2%
1	D	333	 78% 18% 2% 2%
1	E	333	 81% 14% 2% 2%

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Mol	Chain	Length	Quality of chain
1	F	333	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into segments: a small red segment at the start, followed by a large green segment labeled '77%', then a yellow segment labeled '18%', and finally a small grey segment at the end. Above the bar is a '%' symbol, and below the bar are two dots '••'.</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15988 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 Drp35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	2520	1609	418	483	10	0	0	0
1	B	321	2511	1604	415	482	10	0	0	0
1	C	323	2526	1612	419	485	10	0	0	0
1	D	321	2512	1603	417	482	10	0	0	0
1	E	321	2511	1604	416	481	10	0	0	0
1	F	320	2502	1599	414	479	10	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q99QV3
A	2	ALA	-	cloning artifact	UNP Q99QV3
A	138	ASN	ASP	engineered mutation	UNP Q99QV3
A	326	LEU	-	expression tag	UNP Q99QV3
A	327	GLU	-	expression tag	UNP Q99QV3
A	328	HIS	-	expression tag	UNP Q99QV3
A	329	HIS	-	expression tag	UNP Q99QV3
A	330	HIS	-	expression tag	UNP Q99QV3
A	331	HIS	-	expression tag	UNP Q99QV3
A	332	HIS	-	expression tag	UNP Q99QV3
A	333	HIS	-	expression tag	UNP Q99QV3
B	1	MET	-	cloning artifact	UNP Q99QV3
B	2	ALA	-	cloning artifact	UNP Q99QV3
B	138	ASN	ASP	engineered mutation	UNP Q99QV3
B	326	LEU	-	expression tag	UNP Q99QV3
B	327	GLU	-	expression tag	UNP Q99QV3
B	328	HIS	-	expression tag	UNP Q99QV3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	329	HIS	-	expression tag	UNP Q99QV3
B	330	HIS	-	expression tag	UNP Q99QV3
B	331	HIS	-	expression tag	UNP Q99QV3
B	332	HIS	-	expression tag	UNP Q99QV3
B	333	HIS	-	expression tag	UNP Q99QV3
C	1	MET	-	cloning artifact	UNP Q99QV3
C	2	ALA	-	cloning artifact	UNP Q99QV3
C	138	ASN	ASP	engineered mutation	UNP Q99QV3
C	326	LEU	-	expression tag	UNP Q99QV3
C	327	GLU	-	expression tag	UNP Q99QV3
C	328	HIS	-	expression tag	UNP Q99QV3
C	329	HIS	-	expression tag	UNP Q99QV3
C	330	HIS	-	expression tag	UNP Q99QV3
C	331	HIS	-	expression tag	UNP Q99QV3
C	332	HIS	-	expression tag	UNP Q99QV3
C	333	HIS	-	expression tag	UNP Q99QV3
D	1	MET	-	cloning artifact	UNP Q99QV3
D	2	ALA	-	cloning artifact	UNP Q99QV3
D	138	ASN	ASP	engineered mutation	UNP Q99QV3
D	326	LEU	-	expression tag	UNP Q99QV3
D	327	GLU	-	expression tag	UNP Q99QV3
D	328	HIS	-	expression tag	UNP Q99QV3
D	329	HIS	-	expression tag	UNP Q99QV3
D	330	HIS	-	expression tag	UNP Q99QV3
D	331	HIS	-	expression tag	UNP Q99QV3
D	332	HIS	-	expression tag	UNP Q99QV3
D	333	HIS	-	expression tag	UNP Q99QV3
E	1	MET	-	cloning artifact	UNP Q99QV3
E	2	ALA	-	cloning artifact	UNP Q99QV3
E	138	ASN	ASP	engineered mutation	UNP Q99QV3
E	326	LEU	-	expression tag	UNP Q99QV3
E	327	GLU	-	expression tag	UNP Q99QV3
E	328	HIS	-	expression tag	UNP Q99QV3
E	329	HIS	-	expression tag	UNP Q99QV3
E	330	HIS	-	expression tag	UNP Q99QV3
E	331	HIS	-	expression tag	UNP Q99QV3
E	332	HIS	-	expression tag	UNP Q99QV3
E	333	HIS	-	expression tag	UNP Q99QV3
F	1	MET	-	cloning artifact	UNP Q99QV3
F	2	ALA	-	cloning artifact	UNP Q99QV3
F	138	ASN	ASP	engineered mutation	UNP Q99QV3
F	326	LEU	-	expression tag	UNP Q99QV3

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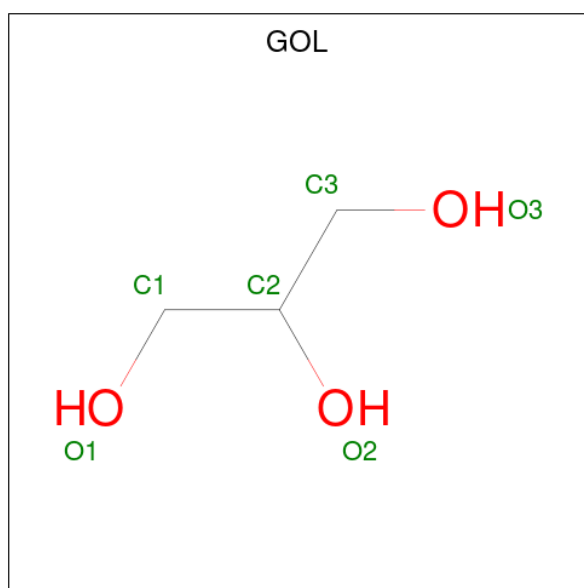
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Chain	Residue	Modelled	Actual	Comment	Reference
F	327	GLU	-	expression tag	UNP Q99QV3
F	328	HIS	-	expression tag	UNP Q99QV3
F	329	HIS	-	expression tag	UNP Q99QV3
F	330	HIS	-	expression tag	UNP Q99QV3
F	331	HIS	-	expression tag	UNP Q99QV3
F	332	HIS	-	expression tag	UNP Q99QV3
F	333	HIS	-	expression tag	UNP Q99QV3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

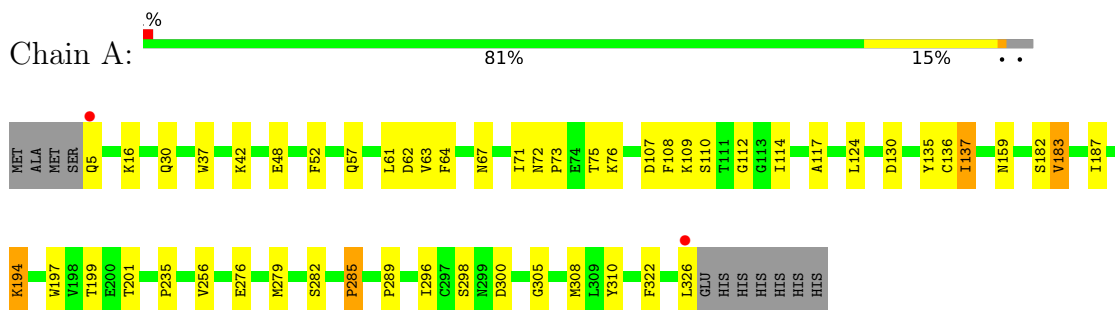
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	143	Total	O	0	0
			143	143		
4	C	124	Total	O	0	0
			124	124		
4	D	145	Total	O	0	0
			145	145		
4	E	170	Total	O	0	0
			170	170		
4	F	139	Total	O	0	0
			139	139		

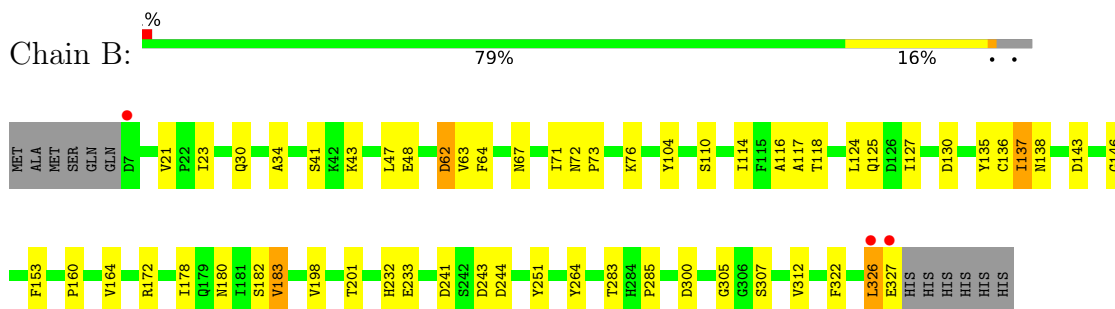
3 Residue-property plots [i](#)

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.

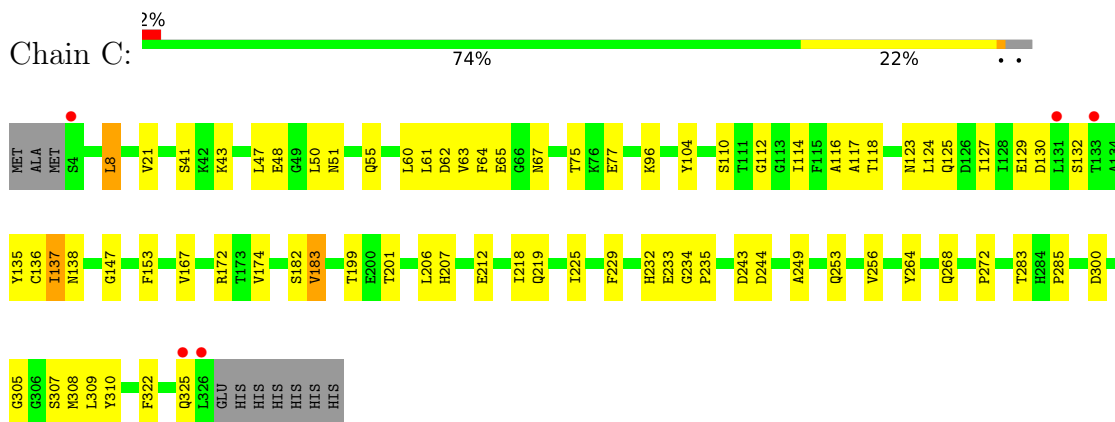
- Molecule 1: Drp35




- Molecule 1: Drp35

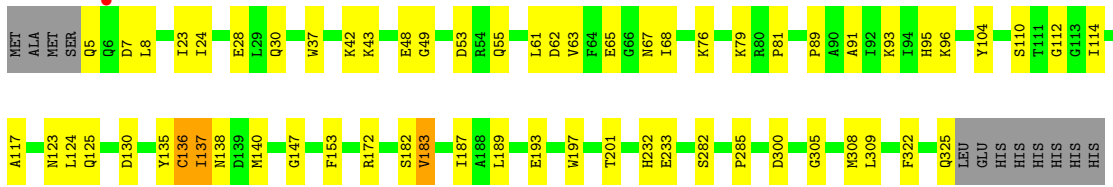


- Molecule 1: Drp35




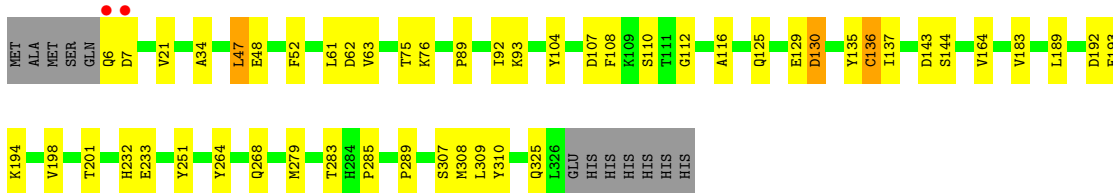
- Molecule 1: Drp35

Chain D:  78% 18%




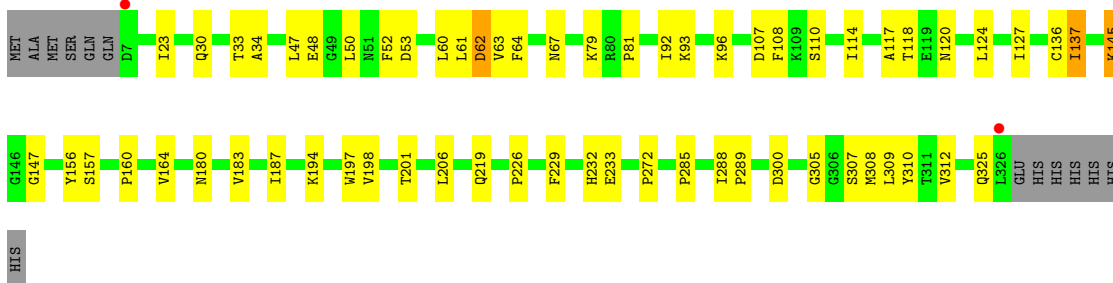
• Molecule 1: Drp35

Chain E:  81% 14%



• Molecule 1: Drp35

Chain F:  77% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.55Å 182.43Å 81.45Å 90.00° 115.58° 90.00°	Depositor
Resolution (Å)	19.99 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.10) 99.6 (19.99-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.168 , 0.202 0.167 , 0.202	Depositor DCC
R_{free} test set	11661 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtrriage
Anisotropy	0.397	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15988	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: CA, GOL

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	0.34	0/2580	0.94	11/3499 (0.3%)
1	B	0.35	0/2571	0.92	10/3487 (0.3%)
1	C	0.34	0/2586	0.94	12/3507 (0.3%)
1	D	0.35	0/2572	0.93	7/3488 (0.2%)
1	E	0.35	0/2571	0.94	6/3487 (0.2%)
1	F	0.35	0/2562	0.94	10/3475 (0.3%)
All	All	0.35	0/15442	0.94	56/20943 (0.3%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	VAL	N-CA-C	9.53	120.37	110.36
1	B	63	VAL	N-CA-C	8.77	118.81	110.30
1	D	63	VAL	N-CA-C	8.73	118.80	110.42
1	E	63	VAL	N-CA-C	8.34	118.39	110.30
1	A	201	THR	N-CA-C	8.24	119.89	111.07
1	B	201	THR	N-CA-C	8.12	119.76	111.07
1	D	201	THR	N-CA-C	8.12	119.82	110.97
1	F	127	ILE	N-CA-C	-7.91	104.16	111.67
1	C	201	THR	N-CA-C	7.46	120.12	111.02
1	A	63	VAL	N-CA-C	7.29	117.42	110.42
1	E	201	THR	N-CA-C	7.24	118.86	110.97
1	C	234	GLY	CA-C-N	7.16	127.14	119.76
1	C	234	GLY	C-N-CA	7.16	127.14	119.76
1	A	130	ASP	N-CA-C	7.11	120.07	111.40
1	C	63	VAL	N-CA-C	6.91	117.00	110.30
1	F	288	ILE	N-CA-C	-6.87	102.22	108.95
1	C	64	PHE	N-CA-C	6.82	119.55	111.71
1	A	322	PHE	N-CA-C	6.66	119.39	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	THR	N-CA-C	6.31	118.72	111.02
1	A	64	PHE	N-CA-C	6.29	119.12	111.82
1	F	137	ILE	N-CA-C	6.19	117.03	107.99
1	C	127	ILE	N-CA-C	-6.15	105.06	111.58
1	F	136	CYS	N-CA-C	-6.12	95.62	107.44
1	A	137	ILE	N-CA-C	5.98	116.72	107.99
1	D	135	TYR	N-CA-C	5.96	118.90	110.50
1	A	159	ASN	CA-C-N	5.89	127.20	119.84
1	A	159	ASN	C-N-CA	5.89	127.20	119.84
1	E	130	ASP	N-CA-C	5.75	118.66	111.24
1	C	8	LEU	N-CA-C	5.67	116.85	109.64
1	E	135	TYR	N-CA-C	5.67	118.50	110.50
1	A	135	TYR	N-CA-C	5.67	118.45	110.23
1	B	118	THR	N-CA-C	-5.66	103.23	110.53
1	E	137	ILE	N-CA-C	5.62	116.20	107.99
1	E	136	CYS	N-CA-C	-5.62	96.59	107.44
1	B	137	ILE	N-CA-C	5.61	116.81	108.23
1	F	147	GLY	N-CA-C	-5.57	103.89	112.85
1	C	212	GLU	N-CA-C	-5.50	103.43	110.53
1	D	30	GLN	N-CA-C	-5.50	101.77	109.96
1	C	137	ILE	N-CA-C	5.50	116.64	108.23
1	A	42	LYS	N-CA-C	-5.46	105.88	112.54
1	B	64	PHE	N-CA-C	5.46	119.20	112.54
1	B	135	TYR	N-CA-C	5.45	118.18	110.50
1	F	30	GLN	N-CA-C	-5.45	101.85	109.96
1	B	30	GLN	N-CA-C	-5.44	101.85	109.96
1	B	127	ILE	N-CA-C	-5.40	106.43	111.45
1	D	136	CYS	N-CA-C	-5.39	97.03	107.44
1	F	118	THR	N-CA-C	-5.36	103.62	110.53
1	C	135	TYR	N-CA-C	5.35	118.19	110.28
1	F	64	PHE	N-CA-C	5.33	119.50	112.89
1	C	283	THR	N-CA-C	5.31	120.41	113.88
1	D	147	GLY	N-CA-C	-5.31	104.48	112.60
1	A	30	GLN	N-CA-C	-5.25	102.14	109.96
1	B	136	CYS	N-CA-C	-5.23	97.34	107.44
1	C	147	GLY	N-CA-C	-5.17	104.53	112.85
1	D	137	ILE	N-CA-C	5.14	115.98	108.58
1	B	143	ASP	N-CA-C	-5.11	103.19	110.59

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2520	0	2446	30	0
1	B	2511	0	2435	31	0
1	C	2526	0	2451	38	0
1	D	2512	0	2434	40	0
1	E	2511	0	2438	26	0
1	F	2502	0	2429	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	6	0	8	0	0
3	D	12	0	16	1	0
4	A	155	0	0	1	0
4	B	143	0	0	0	0
4	C	124	0	0	0	0
4	D	145	0	0	1	0
4	E	170	0	0	0	0
4	F	139	0	0	1	0
All	All	15988	0	14657	192	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 (192) 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:194:LYS:HA	1:A:194:LYS:HE3	1.53	0.90
1:B:326:LEU:HD12	1:B:326:LEU:H	1.38	0.88
1:C:96:LYS:HE2	1:C:325:GLN:HB3	1.57	0.86
1:C:232:HIS:CE1	1:C:233:GLU:HG2	2.18	0.78
1:C:75:THR:OG1	1:C:77:GLU:HG2	1.87	0.75
1:F:194:LYS:HD2	1:F:194:LYS:O	1.87	0.74
1:C:199:THR:HB	1:C:235:PRO:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:SER:OG	1:B:43:LYS:HG2	1.90	0.72
1:C:232:HIS:NE2	1:C:233:GLU:HG2	2.06	0.71
1:E:232:HIS:CE1	1:E:233:GLU:HG3	2.26	0.69
1:C:104:TYR:OH	1:C:130:ASP:HB3	1.93	0.69
1:E:116:ALA:HB3	1:E:125:GLN:HG3	1.75	0.68
1:D:5:GLN:HG3	1:D:7:ASP:H	1.57	0.68
1:D:114:ILE:HG13	1:D:137:ILE:HD12	1.76	0.67
1:E:144:SER:HA	1:E:325:GLN:HE22	1.61	0.65
1:D:232:HIS:CE1	1:D:233:GLU:HG2	2.31	0.65
1:F:194:LYS:HD3	1:F:219:GLN:HE22	1.62	0.65
1:C:41:SER:OG	1:C:43:LYS:HG2	1.98	0.64
1:D:300:ASP:HB3	1:D:305:GLY:HA3	1.80	0.63
1:E:6:GLN:HG2	1:E:7:ASP:H	1.63	0.63
1:C:112:GLY:HA3	1:C:136:CYS:HA	1.81	0.63
1:D:232:HIS:NE2	1:D:233:GLU:HG2	2.14	0.62
1:C:129:GLU:HB3	1:C:132:SER:OG	1.99	0.62
1:A:5:GLN:HE22	1:A:37:TRP:HE1	1.48	0.61
1:F:194:LYS:HD3	1:F:219:GLN:NE2	2.16	0.61
1:B:264:TYR:OH	1:C:253:GLN:HG2	2.00	0.60
1:D:24:ILE:CG1	1:D:28:GLU:HG3	2.31	0.60
1:A:114:ILE:HG13	1:A:137:ILE:HD12	1.83	0.59
1:B:232:HIS:CE1	1:B:233:GLU:HG2	2.38	0.59
1:D:79:LYS:HE2	4:D:5062:HOH:O	2.03	0.59
1:C:62:ASP:OD2	1:C:65:GLU:HB2	2.03	0.58
1:A:279:MET:HE2	1:A:308:MET:HB3	1.84	0.57
1:B:326:LEU:HD12	1:B:326:LEU:N	2.15	0.57
1:B:114:ILE:HG13	1:B:137:ILE:HD12	1.86	0.57
1:F:79:LYS:HE2	4:F:1105:HOH:O	2.03	0.57
1:C:62:ASP:OD1	1:C:67:ASN:HB2	2.05	0.57
1:E:232:HIS:NE2	1:E:233:GLU:HG3	2.20	0.57
1:D:43:LYS:HA	1:F:120:ASN:ND2	2.20	0.56
1:E:189:LEU:HD13	1:E:193:GLU:HG2	1.87	0.55
1:D:24:ILE:HG13	1:D:28:GLU:HG3	1.88	0.55
1:A:279:MET:HE3	1:A:298:SER:HB3	1.88	0.55
1:B:300:ASP:HB3	1:B:305:GLY:HA3	1.90	0.54
1:D:5:GLN:HB3	1:D:8:LEU:HG	1.89	0.54
1:B:104:TYR:OH	1:B:130:ASP:HB3	2.08	0.54
1:F:96:LYS:HD2	1:F:325:GLN:OE1	2.08	0.54
1:D:189:LEU:HD13	1:D:193:GLU:HG2	1.91	0.53
1:E:6:GLN:CD	1:E:6:GLN:N	2.65	0.53
1:B:326:LEU:H	1:B:326:LEU:CD1	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:HB2	1:A:124:LEU:HD13	1.90	0.53
1:E:75:THR:O	1:E:76:LYS:HB2	2.08	0.53
1:D:43:LYS:HA	1:F:120:ASN:HD22	1.73	0.53
1:D:68:ILE:O	1:D:81:PRO:HD2	2.09	0.53
1:A:194:LYS:HA	1:A:194:LYS:CE	2.32	0.52
1:B:116:ALA:HB3	1:B:125:GLN:HG3	1.92	0.52
1:F:232:HIS:CE1	1:F:233:GLU:HG2	2.43	0.52
1:D:23:ILE:HB	3:D:5003:GOL:H31	1.92	0.52
1:C:308:MET:HG3	1:C:309:LEU:N	2.24	0.52
1:A:112:GLY:HA3	1:A:136:CYS:HA	1.91	0.52
1:B:232:HIS:NE2	1:B:233:GLU:HG2	2.25	0.51
1:C:118:THR:CG2	1:C:123:ASN:HD22	2.23	0.51
1:A:109:LYS:HA	1:A:109:LYS:HE2	1.92	0.51
1:C:55:GLN:NE2	1:C:55:GLN:HA	2.26	0.51
1:F:308:MET:HG3	1:F:309:LEU:N	2.24	0.51
1:D:117:ALA:HB2	1:D:124:LEU:HD23	1.93	0.51
1:F:145:LYS:HB2	1:F:145:LYS:NZ	2.25	0.51
1:D:104:TYR:OH	1:D:130:ASP:HB3	2.11	0.51
1:E:164:VAL:HG21	1:E:198:VAL:HG21	1.92	0.51
1:A:199:THR:HB	1:A:235:PRO:HB2	1.92	0.51
1:C:55:GLN:HA	1:C:55:GLN:HE21	1.76	0.51
1:F:232:HIS:NE2	1:F:233:GLU:HG2	2.25	0.50
1:D:96:LYS:HE2	1:D:322:PHE:CE1	2.47	0.50
1:E:61:LEU:HD22	1:E:89:PRO:HB2	1.94	0.50
1:D:232:HIS:CD2	1:D:233:GLU:HG2	2.47	0.49
1:A:57:GLN:OE1	1:A:72:ASN:HA	2.12	0.49
1:A:279:MET:CE	1:A:310:TYR:HE1	2.25	0.49
1:F:114:ILE:HG13	1:F:137:ILE:HD12	1.95	0.49
1:A:75:THR:O	1:A:76:LYS:HB2	2.12	0.48
1:A:61:LEU:HD12	1:A:61:LEU:C	2.39	0.48
1:B:164:VAL:HG21	1:B:198:VAL:HG21	1.95	0.48
1:B:251:TYR:HD1	1:B:283:THR:HG22	1.79	0.48
1:C:206:LEU:HB2	1:C:229:PHE:CE2	2.49	0.48
1:F:62:ASP:OD2	1:F:67:ASN:HB2	2.13	0.48
1:A:276:GLU:N	1:A:276:GLU:OE1	2.47	0.48
1:B:160:PRO:HB2	1:B:180:ASN:C	2.38	0.48
1:C:172:ARG:HH21	1:D:172:ARG:NH1	2.12	0.47
1:F:47:LEU:HD11	1:F:307:SER:HB3	1.97	0.47
1:A:279:MET:CE	1:A:308:MET:HB3	2.44	0.47
1:C:207:HIS:CE1	1:C:225:ILE:HD11	2.50	0.47
1:E:6:GLN:HG2	1:E:7:ASP:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:C	1:D:61:LEU:HD12	2.40	0.47
1:F:206:LEU:HB2	1:F:229:PHE:CE2	2.49	0.47
1:B:251:TYR:CD1	1:B:283:THR:HG22	2.49	0.47
1:F:206:LEU:O	1:F:226:PRO:HD2	2.15	0.47
1:B:23:ILE:HD13	1:C:268:GLN:OE1	2.15	0.47
1:F:232:HIS:CD2	1:F:233:GLU:HG2	2.49	0.47
1:E:104:TYR:OH	1:E:130:ASP:HB3	2.15	0.47
1:A:300:ASP:HB3	1:A:305:GLY:HA3	1.97	0.47
1:A:326:LEU:HD22	1:A:326:LEU:N	2.31	0.47
1:B:21:VAL:HG12	1:B:264:TYR:CE2	2.50	0.47
1:F:164:VAL:HG21	1:F:198:VAL:HG21	1.96	0.47
1:C:232:HIS:CD2	1:C:233:GLU:HG2	2.50	0.46
1:C:117:ALA:HB2	1:C:124:LEU:HD23	1.98	0.46
1:B:172:ARG:HH21	1:B:172:ARG:HB3	1.81	0.46
1:B:182:SER:O	1:B:183:VAL:HB	2.16	0.46
1:C:272:PRO:HD2	1:C:310:TYR:CE2	2.51	0.45
1:F:300:ASP:HB3	1:F:305:GLY:HA3	1.99	0.45
1:A:124:LEU:H	1:A:124:LEU:HD22	1.81	0.45
1:C:249:ALA:HA	1:C:256:VAL:HG22	1.98	0.45
1:D:123:ASN:O	1:D:125:GLN:HG3	2.16	0.45
1:C:300:ASP:HB3	1:C:305:GLY:HA3	1.99	0.45
1:D:95:HIS:ND1	1:D:96:LYS:N	2.64	0.45
1:F:61:LEU:C	1:F:61:LEU:HD12	2.42	0.45
1:F:117:ALA:HB2	1:F:124:LEU:HD23	1.97	0.45
1:C:50:LEU:HD23	1:C:60:LEU:HB3	1.99	0.45
1:C:61:LEU:C	1:C:61:LEU:HD12	2.43	0.44
1:A:124:LEU:HD22	1:A:124:LEU:N	2.32	0.44
1:E:112:GLY:HA3	1:E:136:CYS:HA	1.98	0.44
1:E:279:MET:HG3	1:E:310:TYR:OH	2.18	0.44
1:A:182:SER:O	1:A:183:VAL:HB	2.18	0.44
1:B:326:LEU:HB2	1:B:327:GLU:OE2	2.17	0.44
1:C:47:LEU:HD11	1:C:307:SER:HB3	1.99	0.44
1:D:62:ASP:OD2	1:D:67:ASN:HB2	2.18	0.44
1:D:96:LYS:NZ	1:D:325:GLN:HB2	2.33	0.44
1:D:300:ASP:HB3	1:D:305:GLY:CA	2.48	0.44
1:A:279:MET:HE2	1:A:310:TYR:HE1	1.82	0.44
1:D:93:LYS:HE2	1:D:140:MET:O	2.18	0.44
1:F:160:PRO:HB2	1:F:180:ASN:C	2.42	0.44
1:C:167:VAL:HG22	1:C:174:VAL:HG22	2.00	0.44
1:D:182:SER:O	1:D:183:VAL:HB	2.18	0.44
1:A:62:ASP:OD2	1:A:67:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:OD2	1:D:53:ASP:C	2.61	0.43
1:D:308:MET:HG3	1:D:309:LEU:N	2.33	0.43
1:D:42:LYS:HD2	1:F:81:PRO:HA	2.00	0.43
1:A:256:VAL:HG21	1:A:296:ILE:HD13	2.00	0.43
1:D:37:TRP:CE2	1:D:76:LYS:HE2	2.52	0.43
1:D:138:ASN:HB2	1:D:153:PHE:HB2	2.00	0.43
1:D:187:ILE:HA	1:D:197:TRP:O	2.17	0.43
1:B:34:ALA:HA	1:B:312:VAL:CG1	2.49	0.43
1:B:47:LEU:HD11	1:B:307:SER:HB3	1.99	0.43
1:E:192:ASP:OD1	1:E:194:LYS:HD2	2.19	0.43
1:E:21:VAL:HG12	1:E:264:TYR:CE2	2.54	0.43
1:F:308:MET:HG2	1:F:310:TYR:CZ	2.54	0.43
1:C:96:LYS:HZ3	1:C:325:GLN:HG2	1.84	0.43
1:A:107:ASP:O	1:A:108:PHE:HB2	2.19	0.42
1:B:71:ILE:O	1:B:73:PRO:HD3	2.18	0.42
1:E:92:ILE:O	1:E:93:LYS:HD2	2.18	0.42
1:E:47:LEU:HD22	1:E:307:SER:HB3	2.00	0.42
1:B:72:ASN:O	1:B:76:LYS:N	2.49	0.42
1:B:164:VAL:HB	1:B:178:ILE:HG22	2.02	0.42
1:B:243:ASP:O	1:B:244:ASP:HB2	2.20	0.42
1:C:243:ASP:O	1:C:244:ASP:HB2	2.20	0.42
1:D:112:GLY:HA3	1:D:136:CYS:HA	2.00	0.42
1:B:138:ASN:HB2	1:B:153:PHE:HB2	2.02	0.42
1:F:52:PHE:CG	1:F:289:PRO:HD3	2.54	0.42
1:C:114:ILE:HG13	1:C:137:ILE:HD12	2.02	0.42
1:C:116:ALA:HB3	1:C:125:GLN:HG3	2.01	0.42
1:A:16:LYS:NZ	4:A:5097:HOH:O	2.51	0.42
1:A:52:PHE:CG	1:A:289:PRO:HD3	2.55	0.42
1:A:187:ILE:HA	1:A:197:TRP:O	2.20	0.42
1:C:96:LYS:HE3	1:C:322:PHE:CE1	2.54	0.42
1:E:251:TYR:CD1	1:E:283:THR:HG22	2.54	0.42
1:F:187:ILE:HA	1:F:197:TRP:O	2.19	0.42
1:E:268:GLN:OE1	1:F:23:ILE:HD13	2.20	0.41
1:E:308:MET:HG3	1:E:309:LEU:N	2.35	0.41
1:F:53:ASP:OD2	1:F:53:ASP:C	2.63	0.41
1:F:33:THR:CG2	1:F:272:PRO:HG3	2.50	0.41
1:A:71:ILE:O	1:A:73:PRO:HD3	2.20	0.41
1:C:138:ASN:HB2	1:C:153:PHE:HB2	2.03	0.41
1:D:49:GLY:HA3	1:D:91:ALA:HA	2.02	0.41
1:F:107:ASP:O	1:F:108:PHE:HB2	2.20	0.41
1:C:218:ILE:HG22	1:C:219:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD22	1:D:89:PRO:HB2	2.03	0.41
1:A:279:MET:HE2	1:A:310:TYR:CE1	2.55	0.41
1:E:6:GLN:N	1:E:6:GLN:NE2	2.68	0.41
1:C:182:SER:O	1:C:183:VAL:HB	2.20	0.41
1:D:62:ASP:OD1	1:D:65:GLU:HB2	2.20	0.41
1:E:107:ASP:O	1:E:108:PHE:HB2	2.21	0.41
1:E:143:ASP:OD2	1:E:143:ASP:C	2.64	0.41
1:F:34:ALA:HA	1:F:312:VAL:CG1	2.50	0.41
1:F:50:LEU:HD23	1:F:60:LEU:HB3	2.01	0.41
1:B:117:ALA:HB2	1:B:124:LEU:HD23	2.02	0.41
1:B:62:ASP:OD2	1:B:67:ASN:HB2	2.21	0.41
1:C:21:VAL:HG12	1:C:264:TYR:CE2	2.56	0.41
1:E:52:PHE:CG	1:E:289:PRO:HD3	2.56	0.41
1:E:34:ALA:HB1	1:E:310:TYR:HB3	2.01	0.41
1:F:92:ILE:O	1:F:93:LYS:HD2	2.20	0.41
1:B:146:GLY:HA2	1:B:322:PHE:CZ	2.55	0.40
1:D:96:LYS:HZ3	1:D:325:GLN:HB2	1.86	0.40
1:B:241:ASP:OD2	1:B:241:ASP:C	2.64	0.40
1:F:156:TYR:O	1:F:157:SER:C	2.64	0.40
1:D:42:LYS:CD	1:F:81:PRO:HA	2.52	0.40
1:D:114:ILE:HD11	1:D:137:ILE:HG21	2.04	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	320/333 (96%)	308 (96%)	9 (3%)	3 (1%)	14 10
1	B	319/333 (96%)	307 (96%)	9 (3%)	3 (1%)	14 10
1	C	321/333 (96%)	308 (96%)	10 (3%)	3 (1%)	14 10
1	D	319/333 (96%)	310 (97%)	6 (2%)	3 (1%)	14 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	319/333 (96%)	310 (97%)	6 (2%)	3 (1%)	14	10
1	F	318/333 (96%)	306 (96%)	9 (3%)	3 (1%)	14	10
All	All	1916/1998 (96%)	1849 (96%)	49 (3%)	18 (1%)	14	10

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	SER
1	C	110	SER
1	D	110	SER
1	E	110	SER
1	F	110	SER
1	A	285	PRO
1	B	110	SER
1	B	183	VAL
1	B	285	PRO
1	C	285	PRO
1	E	183	VAL
1	E	285	PRO
1	A	183	VAL
1	C	183	VAL
1	D	183	VAL
1	D	285	PRO
1	F	183	VAL
1	F	285	PRO

5.3.2 Protein sidechains [i](#)

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	275/285 (96%)	271 (98%)	4 (2%)	57	65
1	B	274/285 (96%)	271 (99%)	3 (1%)	65	74
1	C	276/285 (97%)	273 (99%)	3 (1%)	65	74
1	D	274/285 (96%)	271 (99%)	3 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	274/285 (96%)	270 (98%)	4 (2%)	57	65
1	F	273/285 (96%)	270 (99%)	3 (1%)	65	74
All	All	1646/1710 (96%)	1626 (99%)	20 (1%)	63	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	194	LYS
1	A	282	SER
1	A	285	PRO
1	B	48	GLU
1	B	62	ASP
1	B	326	LEU
1	C	8	LEU
1	C	48	GLU
1	C	51	ASN
1	D	48	GLU
1	D	55	GLN
1	D	282	SER
1	E	47	LEU
1	E	48	GLU
1	E	62	ASP
1	E	129	GLU
1	F	48	GLU
1	F	62	ASP
1	F	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	286	GLN
1	A	313	ASN
1	B	55	GLN
1	B	88	ASN
1	B	179	GLN
1	B	286	GLN
1	B	293	GLN
1	B	313	ASN

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Mol	Chain	Res	Type
1	C	18	ASN
1	C	55	GLN
1	C	123	ASN
1	C	286	GLN
1	C	325	GLN
1	D	286	GLN
1	E	55	GLN
1	E	179	GLN
1	E	232	HIS
1	E	286	GLN
1	E	319	HIS
1	E	325	GLN
1	F	88	ASN
1	F	123	ASN
1	F	159	ASN
1	F	179	GLN
1	F	219	GLN
1	F	286	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 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	$\# Z > 2$
3	GOL	D	5001	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	D	5003	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	A	5002	-	5,5,5	0.32	0	5,5,5	0.28	0

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
3	GOL	D	5001	-	-	0/4/4/4	-
3	GOL	D	5003	-	-	1/4/4/4	-
3	GOL	A	5002	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	5003	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5003	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	322/333 (96%)	-0.45	2 (0%) 85 87	14, 24, 37, 69	0
1	B	321/333 (96%)	-0.45	3 (0%) 81 83	16, 24, 36, 69	0
1	C	323/333 (96%)	-0.29	5 (1%) 72 74	15, 26, 45, 81	0
1	D	321/333 (96%)	-0.54	1 (0%) 90 91	14, 23, 36, 60	0
1	E	321/333 (96%)	-0.54	2 (0%) 85 87	15, 23, 36, 59	0
1	F	320/333 (96%)	-0.49	2 (0%) 85 87	16, 24, 37, 48	0
All	All	1928/1998 (96%)	-0.46	15 (0%) 82 84	14, 24, 39, 81	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	LEU	5.2
1	C	4	SER	4.9
1	F	326	LEU	3.7
1	B	7	ASP	3.5
1	A	326	LEU	3.1
1	B	326	LEU	3.0
1	E	6	GLN	2.8
1	B	327	GLU	2.7
1	A	5	GLN	2.4
1	F	7	ASP	2.4
1	E	7	ASP	2.3
1	C	133	THR	2.2
1	C	325	GLN	2.1
1	D	6	GLN	2.1
1	C	131	LEU	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
3	GOL	D	5003	6/6	0.81	0.16	51,55,57,61	0
3	GOL	A	5002	6/6	0.83	0.12	53,54,56,59	0
3	GOL	D	5001	6/6	0.91	0.10	30,33,34,37	0
2	CA	F	1012	1/1	0.96	0.07	22,22,22,22	1
2	CA	A	1007	1/1	0.97	0.05	25,25,25,25	1
2	CA	E	1011	1/1	0.97	0.04	25,25,25,25	1
2	CA	C	1009	1/1	0.98	0.11	30,30,30,30	1
2	CA	B	1008	1/1	0.98	0.04	26,26,26,26	1
2	CA	F	1006	1/1	0.99	0.02	23,23,23,23	0
2	CA	B	1002	1/1	0.99	0.05	24,24,24,24	0
2	CA	D	1004	1/1	0.99	0.06	22,22,22,22	0
2	CA	D	1010	1/1	0.99	0.03	24,24,24,24	1
2	CA	A	1001	1/1	0.99	0.02	22,22,22,22	0
2	CA	C	1003	1/1	1.00	0.04	22,22,22,22	0
2	CA	E	1005	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.