



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:47 AM UTC

PDB ID : 6GRJ / pdb_00006grj
Title : Structure of the AhlB pore of the tripartite alpha-pore forming toxin, AHL, from *Aeromonas hydrophila*.
Authors : Churchill-Angus, A.M.; Wilson, J.S.; Baker, P.J.
Deposited on : 2018-06-11
Resolution : 2.94 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

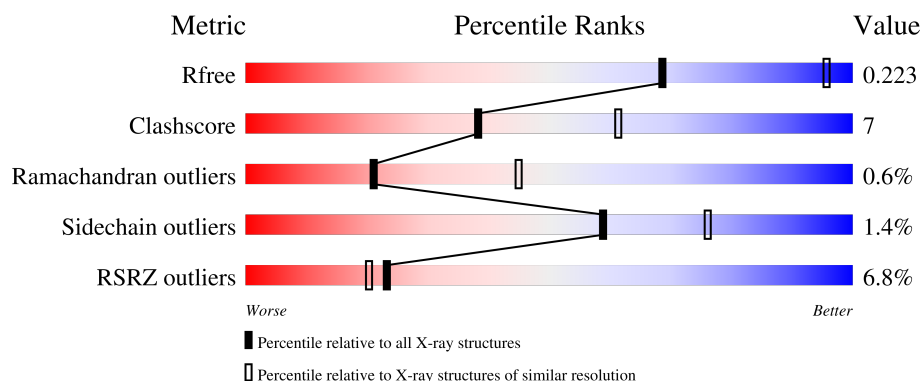
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	367	
1	B	367	
1	C	367	
1	D	367	
1	E	367	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	367	
1	G	367	
1	H	367	
1	I	367	
1	J	367	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NA	C	409	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24385 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 AhlB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	338	Total	C	N	O	S	Se	0	0	0
			2489	1550	431	501	1	6			
1	J	322	Total	C	N	O	S	Se	0	0	0
			2375	1483	412	475	1	4			
1	A	338	Total	C	N	O	S	Se	0	0	0
			2489	1550	431	501	1	6			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2375	1483	412	475	1	4			
1	C	338	Total	C	N	O	S	Se	0	0	0
			2488	1549	431	501	1	6			
1	D	320	Total	C	N	O	S	Se	0	0	0
			2367	1478	411	473	1	4			
1	E	338	Total	C	N	O	S	Se	0	1	0
			2492	1552	432	501	1	6			
1	F	317	Total	C	N	O	S	Se	0	0	0
			2343	1464	406	468	1	4			
1	H	337	Total	C	N	O	S	Se	0	0	0
			2482	1546	430	499	1	6			
1	I	315	Total	C	N	O	S	Se	0	0	0
			2326	1452	405	464	1	4			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	336	ILE	MET	engineered mutation	UNP A0A081US78
G	360	LEU	-	expression tag	UNP A0A081US78
G	361	GLU	-	expression tag	UNP A0A081US78
G	362	HIS	-	expression tag	UNP A0A081US78
G	363	HIS	-	expression tag	UNP A0A081US78
G	364	HIS	-	expression tag	UNP A0A081US78
G	365	HIS	-	expression tag	UNP A0A081US78
G	366	HIS	-	expression tag	UNP A0A081US78
G	367	HIS	-	expression tag	UNP A0A081US78

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	336	ILE	MET	engineered mutation	UNP A0A081US78
J	360	LEU	-	expression tag	UNP A0A081US78
J	361	GLU	-	expression tag	UNP A0A081US78
J	362	HIS	-	expression tag	UNP A0A081US78
J	363	HIS	-	expression tag	UNP A0A081US78
J	364	HIS	-	expression tag	UNP A0A081US78
J	365	HIS	-	expression tag	UNP A0A081US78
J	366	HIS	-	expression tag	UNP A0A081US78
J	367	HIS	-	expression tag	UNP A0A081US78
A	336	ILE	MET	engineered mutation	UNP A0A081US78
A	360	LEU	-	expression tag	UNP A0A081US78
A	361	GLU	-	expression tag	UNP A0A081US78
A	362	HIS	-	expression tag	UNP A0A081US78
A	363	HIS	-	expression tag	UNP A0A081US78
A	364	HIS	-	expression tag	UNP A0A081US78
A	365	HIS	-	expression tag	UNP A0A081US78
A	366	HIS	-	expression tag	UNP A0A081US78
A	367	HIS	-	expression tag	UNP A0A081US78
B	336	ILE	MET	engineered mutation	UNP A0A081US78
B	360	LEU	-	expression tag	UNP A0A081US78
B	361	GLU	-	expression tag	UNP A0A081US78
B	362	HIS	-	expression tag	UNP A0A081US78
B	363	HIS	-	expression tag	UNP A0A081US78
B	364	HIS	-	expression tag	UNP A0A081US78
B	365	HIS	-	expression tag	UNP A0A081US78
B	366	HIS	-	expression tag	UNP A0A081US78
B	367	HIS	-	expression tag	UNP A0A081US78
C	336	ILE	MET	engineered mutation	UNP A0A081US78
C	360	LEU	-	expression tag	UNP A0A081US78
C	361	GLU	-	expression tag	UNP A0A081US78
C	362	HIS	-	expression tag	UNP A0A081US78
C	363	HIS	-	expression tag	UNP A0A081US78
C	364	HIS	-	expression tag	UNP A0A081US78
C	365	HIS	-	expression tag	UNP A0A081US78
C	366	HIS	-	expression tag	UNP A0A081US78
C	367	HIS	-	expression tag	UNP A0A081US78
D	336	ILE	MET	engineered mutation	UNP A0A081US78
D	360	LEU	-	expression tag	UNP A0A081US78
D	361	GLU	-	expression tag	UNP A0A081US78
D	362	HIS	-	expression tag	UNP A0A081US78
D	363	HIS	-	expression tag	UNP A0A081US78
D	364	HIS	-	expression tag	UNP A0A081US78

Continued on next page...

Continued from previous page...

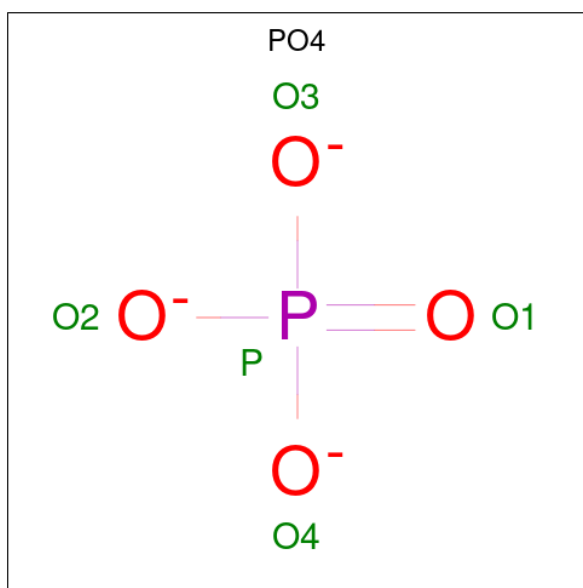
Chain	Residue	Modelled	Actual	Comment	Reference
D	365	HIS	-	expression tag	UNP A0A081US78
D	366	HIS	-	expression tag	UNP A0A081US78
D	367	HIS	-	expression tag	UNP A0A081US78
E	336	ILE	MET	engineered mutation	UNP A0A081US78
E	360	LEU	-	expression tag	UNP A0A081US78
E	361	GLU	-	expression tag	UNP A0A081US78
E	362	HIS	-	expression tag	UNP A0A081US78
E	363	HIS	-	expression tag	UNP A0A081US78
E	364	HIS	-	expression tag	UNP A0A081US78
E	365	HIS	-	expression tag	UNP A0A081US78
E	366	HIS	-	expression tag	UNP A0A081US78
E	367	HIS	-	expression tag	UNP A0A081US78
F	336	ILE	MET	engineered mutation	UNP A0A081US78
F	360	LEU	-	expression tag	UNP A0A081US78
F	361	GLU	-	expression tag	UNP A0A081US78
F	362	HIS	-	expression tag	UNP A0A081US78
F	363	HIS	-	expression tag	UNP A0A081US78
F	364	HIS	-	expression tag	UNP A0A081US78
F	365	HIS	-	expression tag	UNP A0A081US78
F	366	HIS	-	expression tag	UNP A0A081US78
F	367	HIS	-	expression tag	UNP A0A081US78
H	336	ILE	MET	engineered mutation	UNP A0A081US78
H	360	LEU	-	expression tag	UNP A0A081US78
H	361	GLU	-	expression tag	UNP A0A081US78
H	362	HIS	-	expression tag	UNP A0A081US78
H	363	HIS	-	expression tag	UNP A0A081US78
H	364	HIS	-	expression tag	UNP A0A081US78
H	365	HIS	-	expression tag	UNP A0A081US78
H	366	HIS	-	expression tag	UNP A0A081US78
H	367	HIS	-	expression tag	UNP A0A081US78
I	336	ILE	MET	engineered mutation	UNP A0A081US78
I	360	LEU	-	expression tag	UNP A0A081US78
I	361	GLU	-	expression tag	UNP A0A081US78
I	362	HIS	-	expression tag	UNP A0A081US78
I	363	HIS	-	expression tag	UNP A0A081US78
I	364	HIS	-	expression tag	UNP A0A081US78
I	365	HIS	-	expression tag	UNP A0A081US78
I	366	HIS	-	expression tag	UNP A0A081US78
I	367	HIS	-	expression tag	UNP A0A081US78

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	J	1	Total	C	O	0	0
			8	6	2		
2	J	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	H	1	Total	C	O	0	0
			8	6	2		
2	H	1	Total	C	O	0	0
			8	6	2		
2	I	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	3	Total	Cl	0	0
			3	3		
4	J	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	B	2	Total	Cl	0	0
			2	2		
4	C	5	Total	Cl	0	0
			5	5		
4	D	2	Total	Cl	0	0
			2	2		
4	E	2	Total	Cl	0	0
			2	2		
4	F	4	Total	Cl	0	0
			4	4		
4	H	3	Total	Cl	0	0
			3	3		

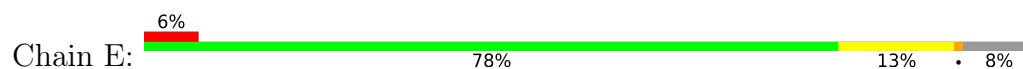
Continued on next page...

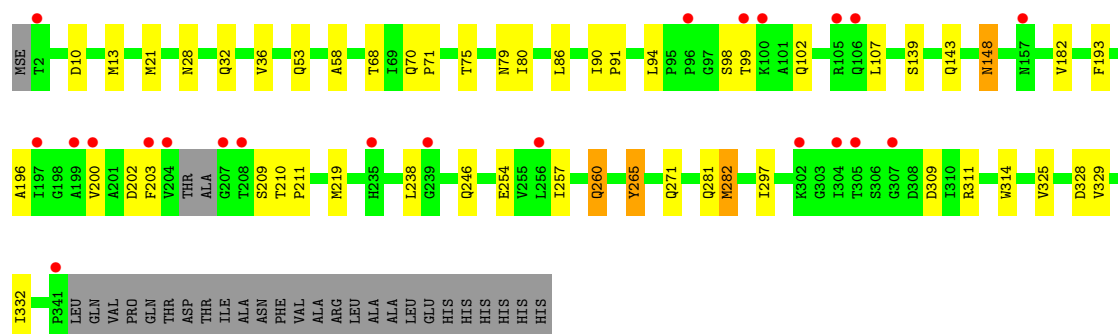
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	4	Total Cl 4 4	0	0

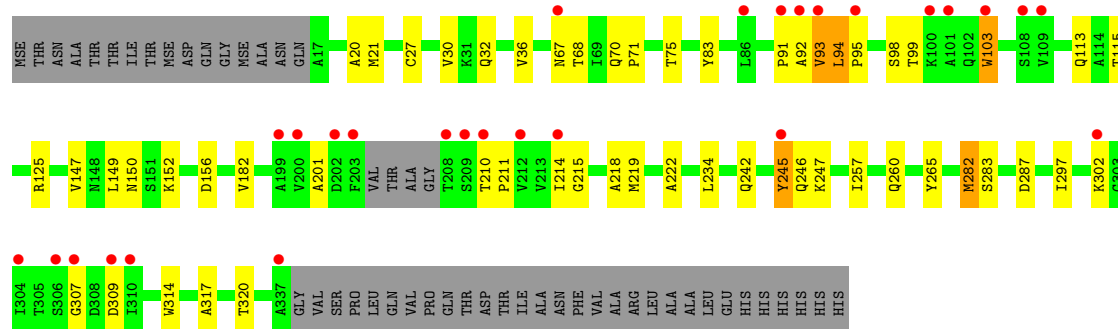
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	3	Total Na 3 3	0	0
5	D	1	Total Na 1 1	0	0
5	E	2	Total Na 2 2	0	0
5	F	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0

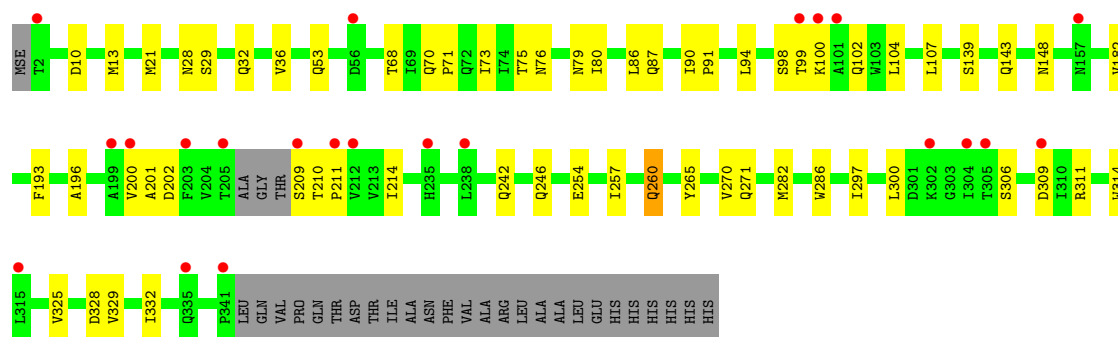
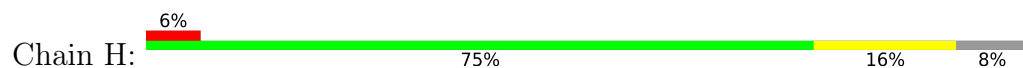




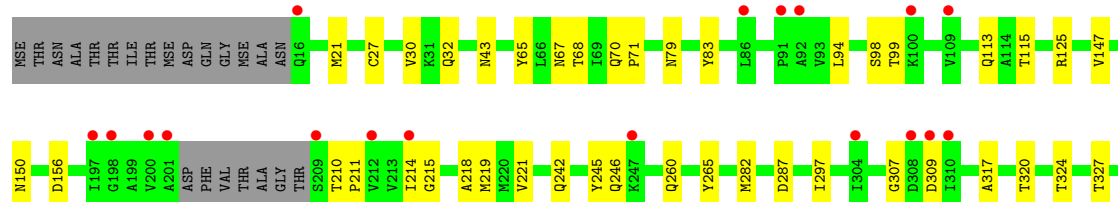
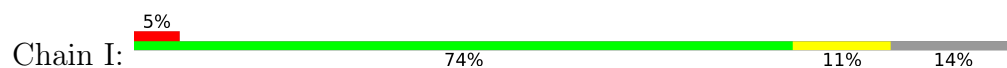
• Molecule 1: AhlB



• Molecule 1: AhlB



• Molecule 1: AhlB



A337
GLY
VAL
SER
PRO
LEU
GLN
VAL
PRO
GLN
THR
ASP
THR
ILE
ALA
ASN
PHE
VAL
ALA
ALA
ARG
LEU
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	363.64Å 116.53Å 217.41Å 90.00° 118.01° 90.00°	Depositor
Resolution (Å)	102.67 – 2.94 102.67 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.9 (102.67-2.94) 98.7 (102.67-2.94)	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	REFMAC 5.8.0222	Depositor
R, R_{free}	0.222 , 0.239 0.231 , 0.223	Depositor DCC
R_{free} test set	8485 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24385	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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: MPD, NA, PO4, CL

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	0.94	5/2509 (0.2%)	1.26	5/3410 (0.1%)
1	B	0.93	3/2397 (0.1%)	1.24	7/3261 (0.2%)
1	C	0.97	4/2508 (0.2%)	1.25	4/3408 (0.1%)
1	D	0.96	5/2388 (0.2%)	1.25	7/3247 (0.2%)
1	E	0.93	5/2515 (0.2%)	1.24	5/3417 (0.1%)
1	F	0.98	6/2364 (0.3%)	1.24	6/3214 (0.2%)
1	G	0.95	6/2509 (0.2%)	1.25	5/3410 (0.1%)
1	H	0.92	5/2502 (0.2%)	1.23	5/3400 (0.1%)
1	I	0.94	2/2346 (0.1%)	1.22	8/3189 (0.3%)
1	J	0.97	7/2397 (0.3%)	1.26	8/3261 (0.2%)
All	All	0.95	48/24435 (0.2%)	1.24	60/33217 (0.2%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	GLN	C-O	-9.03	1.13	1.24
1	C	260	GLN	C-O	-8.83	1.13	1.24
1	H	260	GLN	C-O	-8.58	1.14	1.24
1	G	260	GLN	C-O	-8.49	1.14	1.24
1	E	260	GLN	C-O	-8.31	1.14	1.24
1	D	79	ASN	C-O	7.55	1.32	1.24
1	F	93	VAL	C-O	-7.22	1.16	1.23
1	A	79	ASN	C-O	-6.72	1.16	1.24
1	F	182	VAL	C-O	-6.63	1.16	1.24
1	J	182	VAL	C-O	-6.49	1.16	1.24
1	E	182	VAL	C-O	6.47	1.31	1.24
1	C	79	ASN	C-O	-6.45	1.16	1.24
1	E	79	ASN	C-O	-6.39	1.16	1.24
1	A	75	THR	C-O	-6.36	1.16	1.24
1	A	158	GLY	C-O	-6.33	1.15	1.23
1	J	79	ASN	C-O	6.25	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	ASN	C-O	6.22	1.31	1.24
1	G	79	ASN	C-O	-6.15	1.17	1.24
1	H	79	ASN	C-O	-6.15	1.17	1.24
1	I	79	ASN	C-O	6.14	1.31	1.24
1	F	260	GLN	C-O	6.09	1.31	1.24
1	H	182	VAL	C-O	5.94	1.30	1.24
1	I	260	GLN	C-O	5.89	1.30	1.24
1	H	75	THR	C-O	-5.86	1.17	1.24
1	G	158	GLY	C-O	-5.82	1.16	1.23
1	B	260	GLN	C-O	5.63	1.30	1.24
1	E	75	THR	C-O	-5.62	1.17	1.24
1	J	197	ILE	C-O	-5.60	1.17	1.24
1	J	260	GLN	C-O	5.56	1.30	1.24
1	D	245	TYR	C-O	-5.52	1.16	1.24
1	D	234	LEU	C-O	-5.49	1.17	1.24
1	C	158	GLY	C-O	-5.48	1.16	1.23
1	G	53	GLN	C-O	-5.48	1.17	1.24
1	G	75	THR	C-O	-5.47	1.17	1.24
1	C	75	THR	C-O	-5.42	1.17	1.24
1	F	234	LEU	C-O	-5.38	1.17	1.24
1	J	245	TYR	C-O	-5.36	1.17	1.24
1	J	234	LEU	C-O	-5.33	1.18	1.24
1	B	234	LEU	C-O	-5.29	1.18	1.24
1	A	53	GLN	C-O	-5.28	1.17	1.24
1	D	75	THR	C-O	5.28	1.30	1.24
1	H	53	GLN	C-O	-5.22	1.18	1.24
1	D	260	GLN	C-O	5.18	1.30	1.24
1	G	182	VAL	C-O	5.15	1.29	1.24
1	F	201	ALA	CA-CB	-5.12	1.46	1.53
1	J	75	THR	C-O	5.05	1.29	1.24
1	E	53	GLN	C-O	-5.05	1.18	1.24
1	F	75	THR	C-O	5.02	1.29	1.24

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	282	MSE	CG-SE-CE	-8.69	79.81	98.92
1	I	282	MSE	CG-SE-CE	-7.53	82.36	98.92
1	E	21	MSE	CG-SE-CE	7.50	115.43	98.92
1	A	193	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	21	MSE	CG-SE-CE	7.02	114.38	98.92
1	G	21	MSE	CG-SE-CE	7.00	114.32	98.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	MSE	CG-SE-CE	-7.00	83.53	98.92
1	E	193	PHE	CA-CB-CG	6.92	120.72	113.80
1	H	21	MSE	CG-SE-CE	6.87	114.03	98.92
1	C	193	PHE	CA-CB-CG	6.82	120.62	113.80
1	D	282	MSE	CG-SE-CE	-6.56	84.48	98.92
1	F	150	ASN	CA-CB-CG	-6.19	106.41	112.60
1	J	203	PHE	CA-CB-CG	6.05	119.85	113.80
1	I	219	MSE	CG-SE-CE	-6.03	85.66	98.92
1	D	320	THR	CA-C-O	5.99	126.77	120.42
1	D	150	ASN	CA-CB-CG	-5.88	106.72	112.60
1	G	193	PHE	CA-CB-CG	5.84	119.64	113.80
1	F	265	TYR	CB-CA-C	5.78	120.67	110.85
1	J	265	TYR	CB-CA-C	5.68	120.51	110.85
1	J	309	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	320	THR	CA-C-O	5.64	126.40	120.42
1	B	265	TYR	CB-CA-C	5.62	120.40	110.85
1	J	320	THR	CA-C-O	5.60	126.36	120.42
1	I	265	TYR	CB-CA-C	5.60	120.36	110.85
1	A	201	ALA	N-CA-C	-5.57	107.13	114.31
1	F	219	MSE	CG-SE-CE	-5.54	86.74	98.92
1	I	150	ASN	CA-CB-CG	-5.53	107.07	112.60
1	D	265	TYR	CB-CA-C	5.52	120.23	110.85
1	F	245	TYR	CA-CB-CG	5.52	123.83	113.90
1	J	150	ASN	CA-CB-CG	-5.47	107.13	112.60
1	F	320	THR	CA-C-O	5.47	126.22	120.42
1	C	201	ALA	N-CA-C	-5.40	107.34	114.31
1	I	320	THR	CA-C-O	5.40	126.14	120.42
1	A	148	ASN	CB-CA-C	5.36	119.96	110.85
1	D	245	TYR	CA-CB-CG	5.33	123.49	113.90
1	B	150	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	309	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	309	ASP	CA-CB-CG	5.32	117.92	112.60
1	I	245	TYR	CA-CB-CG	5.32	123.47	113.90
1	G	309	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	309	ASP	CA-CB-CG	5.26	117.86	112.60
1	H	21	MSE	CB-CG-SE	-5.20	97.11	112.70
1	J	201	ALA	N-CA-C	-5.18	107.62	114.31
1	D	201	ALA	N-CA-C	-5.16	107.65	114.31
1	F	309	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	148	ASN	CB-CA-C	5.15	119.61	110.85
1	E	219	MSE	CG-SE-CE	-5.14	87.60	98.92
1	I	309	ASP	CA-CB-CG	5.14	117.74	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	201	ALA	N-CA-C	-5.10	107.73	114.31
1	G	201	ALA	N-CA-C	-5.08	107.76	114.31
1	B	309	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	21	MSE	CB-CG-SE	-5.08	97.47	112.70
1	H	193	PHE	CA-CB-CG	5.05	118.85	113.80
1	J	245	TYR	CA-CB-CG	5.05	122.99	113.90
1	D	309	ASP	CA-CB-CG	5.04	117.64	112.60
1	I	265	TYR	CA-C-O	-5.04	115.08	120.42
1	B	203	PHE	N-CA-C	-5.03	107.19	113.38
1	C	309	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	245	TYR	CA-CB-CG	5.01	122.92	113.90
1	C	148	ASN	CB-CA-C	5.00	119.35	110.85

There are no chirality outliers.

There are no planarity outliers.

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	2489	0	2515	39	0
1	B	2375	0	2405	37	0
1	C	2488	0	2511	52	0
1	D	2367	0	2396	25	0
1	E	2492	0	2519	40	0
1	F	2343	0	2372	45	0
1	G	2489	0	2515	42	0
1	H	2482	0	2508	43	0
1	I	2326	0	2361	24	0
1	J	2375	0	2406	44	0
2	A	8	0	14	0	0
2	C	16	0	28	3	0
2	E	16	0	28	4	0
2	F	8	0	14	3	0
2	G	24	0	42	0	0
2	H	16	0	28	3	0
2	I	8	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	16	0	28	1	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	3	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	1	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	4	0	0	0	0
4	J	1	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
All	All	24385	0	24704	339	0

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

All (339) 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:C:13:MSE:HA	1:C:282:MSE:CE	1.89	1.03
1:C:13:MSE:N	1:C:282:MSE:HE2	1.79	0.97
1:C:12:GLY:C	1:C:282:MSE:HE2	1.90	0.97
1:E:260:GLN:HG3	2:E:401:MPD:H52	1.42	0.96
1:C:13:MSE:HA	1:C:282:MSE:HE3	1.46	0.96
1:C:13:MSE:CA	1:C:282:MSE:CE	2.44	0.95
1:C:15:ASN:ND2	1:C:281:GLN:HE22	1.68	0.89
1:C:13:MSE:N	1:C:282:MSE:CE	2.36	0.87
1:A:11:GLN:HG2	1:F:71:PRO:HG3	1.56	0.87
1:J:125:ARG:HD3	1:J:287:ASP:OD1	1.77	0.84
1:F:125:ARG:HD3	1:F:287:ASP:OD1	1.80	0.82
1:J:197:ILE:HD11	1:C:214:ILE:HG23	1.62	0.80
1:B:125:ARG:HD3	1:B:287:ASP:OD1	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ASN:HD22	1:C:281:GLN:HE22	1.27	0.78
1:H:80:ILE:HD11	1:H:282:MSE:CE	2.15	0.77
1:H:260:GLN:HG3	2:H:401:MPD:H52	1.68	0.76
1:C:15:ASN:HD22	1:C:281:GLN:NE2	1.83	0.75
1:H:80:ILE:HD11	1:H:282:MSE:HE1	1.70	0.74
1:D:67:ASN:ND2	1:E:281:GLN:OE1	2.21	0.73
1:C:196:ALA:HB1	1:D:221:VAL:HG12	1.77	0.67
1:J:125:ARG:CD	1:J:287:ASP:OD1	2.43	0.66
1:F:125:ARG:CD	1:F:287:ASP:OD1	2.43	0.66
1:C:13:MSE:CA	1:C:282:MSE:HE2	2.22	0.65
1:I:125:ARG:CD	1:I:287:ASP:OD1	2.44	0.65
1:B:125:ARG:CD	1:B:287:ASP:OD1	2.44	0.65
1:D:125:ARG:CD	1:D:287:ASP:OD1	2.45	0.64
1:B:202:ASP:OD1	1:B:209:SER:HB2	1.97	0.64
1:C:202:ASP:OD1	1:C:209:SER:HB2	1.98	0.64
1:G:202:ASP:OD1	1:G:209:SER:HB2	1.97	0.64
1:J:202:ASP:OD1	1:J:209:SER:HB2	1.98	0.64
1:H:202:ASP:OD1	1:H:209:SER:HB2	1.97	0.64
1:J:205:THR:O	1:J:207:GLY:N	2.31	0.63
1:C:76:ASN:HD21	1:C:286:TRP:HE1	1.45	0.63
1:D:202:ASP:OD1	1:D:209:SER:HB2	1.98	0.63
1:E:202:ASP:OD1	1:E:209:SER:HB2	1.98	0.63
1:B:205:THR:O	1:B:207:GLY:N	2.33	0.62
1:A:202:ASP:OD1	1:A:209:SER:HB2	1.99	0.61
1:C:238:LEU:HD22	4:C:407:CL:CL	2.37	0.61
1:E:86:LEU:HD23	1:F:317:ALA:HB2	1.82	0.61
1:J:197:ILE:HD11	1:C:214:ILE:CG2	2.29	0.61
1:A:196:ALA:HB1	1:B:221:VAL:HG12	1.83	0.61
1:I:125:ARG:HD3	1:I:287:ASP:OD1	2.00	0.61
1:J:143:GLN:OE1	1:J:266:LYS:NZ	2.33	0.60
1:H:246:GLN:NE2	1:I:156:ASP:OD1	2.34	0.60
1:B:205:THR:O	1:B:206:ALA:C	2.44	0.60
1:G:246:GLN:NE2	1:J:156:ASP:OD1	2.34	0.59
1:F:94:LEU:HA	1:F:103:TRP:CE3	2.37	0.59
1:D:125:ARG:HD3	1:D:287:ASP:OD1	2.01	0.59
1:E:107:LEU:CB	1:E:297:ILE:HD11	2.33	0.59
1:J:204:VAL:HG12	1:J:204:VAL:O	2.03	0.58
1:A:86:LEU:HD23	1:B:317:ALA:HB2	1.84	0.58
1:A:80:ILE:HD11	1:A:282:MSE:CE	2.34	0.58
1:F:95:PRO:HD3	1:F:103:TRP:CE3	2.39	0.58
1:A:107:LEU:HB3	1:A:297:ILE:HD11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:SER:HB3	1:E:102:GLN:OE1	2.04	0.58
1:C:107:LEU:HB3	1:C:297:ILE:HD11	1.84	0.58
1:E:107:LEU:HB3	1:E:297:ILE:HD11	1.86	0.58
1:G:76:ASN:HD21	1:G:286:TRP:HE1	1.51	0.57
1:G:98:SER:HB3	1:G:102:GLN:OE1	2.05	0.57
1:H:98:SER:HB3	1:H:102:GLN:OE1	2.04	0.57
1:A:107:LEU:CB	1:A:297:ILE:HD11	2.35	0.57
1:B:197:ILE:HG21	1:H:214:ILE:HD12	1.86	0.57
1:C:98:SER:HB3	1:C:102:GLN:OE1	2.05	0.57
1:C:107:LEU:CB	1:C:297:ILE:HD11	2.35	0.56
1:B:125:ARG:NH1	1:B:283:SER:HB3	2.20	0.56
1:H:28:ASN:O	1:H:32:GLN:HG3	2.04	0.56
1:J:205:THR:O	1:J:206:ALA:C	2.48	0.56
1:D:204:VAL:HG12	1:D:204:VAL:O	2.06	0.56
1:A:28:ASN:O	1:A:32:GLN:HG3	2.05	0.56
1:G:107:LEU:CB	1:G:297:ILE:HD11	2.36	0.56
1:G:107:LEU:HB3	1:G:297:ILE:HD11	1.87	0.56
1:J:83:TYR:CE1	1:J:113:GLN:HG2	2.42	0.55
1:G:28:ASN:O	1:G:32:GLN:HG3	2.06	0.55
1:G:204:VAL:HG12	1:G:204:VAL:O	2.06	0.55
1:C:28:ASN:O	1:C:32:GLN:HG3	2.06	0.55
1:F:83:TYR:CE1	1:F:113:GLN:HG2	2.42	0.55
1:G:13:MSE:SE	1:G:329:VAL:HG22	2.57	0.55
1:H:260:GLN:CG	2:H:401:MPD:H52	2.35	0.55
1:E:28:ASN:O	1:E:32:GLN:HG3	2.06	0.55
1:H:107:LEU:HB3	1:H:297:ILE:HD11	1.88	0.55
1:H:107:LEU:CB	1:H:297:ILE:HD11	2.36	0.55
1:D:83:TYR:CE1	1:D:113:GLN:HG2	2.42	0.55
1:C:13:MSE:SE	1:C:329:VAL:HG22	2.58	0.54
1:G:238:LEU:HD13	1:J:247:LYS:HD2	1.89	0.54
1:I:83:TYR:CE1	1:I:113:GLN:HG2	2.43	0.54
1:F:125:ARG:NH1	1:F:283:SER:HB3	2.21	0.54
1:D:181:ILE:HG21	2:E:402:MPD:HM3	1.89	0.54
1:E:80:ILE:HD11	1:E:282:MSE:CE	2.37	0.54
1:B:83:TYR:CE1	1:B:113:GLN:HG2	2.43	0.54
1:E:238:LEU:CD1	1:F:247:LYS:HE3	2.37	0.54
1:F:91:PRO:HB2	1:F:103:TRP:HZ3	1.73	0.53
1:A:160:LEU:HD21	1:A:164:ASN:HD21	1.74	0.53
1:F:91:PRO:O	1:F:103:TRP:CH2	2.62	0.53
1:E:139:SER:O	1:E:143:GLN:HG2	2.08	0.53
1:G:139:SER:O	1:G:143:GLN:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ASN:HD22	1:C:281:GLN:CD	2.16	0.53
1:A:80:ILE:HD11	1:A:282:MSE:HE1	1.91	0.53
1:B:94:LEU:HD21	1:B:98:SER:O	2.09	0.52
1:A:11:GLN:OE1	1:F:70:GLN:NE2	2.32	0.52
1:A:328:ASP:O	1:A:332:ILE:HG13	2.09	0.52
1:C:3:ASN:HB3	4:C:403:CL:CL	2.47	0.52
1:B:197:ILE:HG21	1:H:214:ILE:CD1	2.39	0.52
1:H:76:ASN:HD21	1:H:286:TRP:HE1	1.56	0.52
1:A:139:SER:O	1:A:143:GLN:HG2	2.10	0.52
1:H:13:MSE:SE	1:H:329:VAL:HG22	2.60	0.52
1:C:139:SER:O	1:C:143:GLN:HG2	2.10	0.52
1:H:80:ILE:HD11	1:H:282:MSE:HE2	1.90	0.52
1:G:257:ILE:HD11	1:J:147:VAL:HG11	1.93	0.51
1:H:328:ASP:O	1:H:332:ILE:HG13	2.10	0.51
1:I:94:LEU:HD23	1:I:94:LEU:C	2.36	0.51
1:C:13:MSE:HA	1:C:282:MSE:HE2	1.81	0.51
1:H:100:LYS:CE	1:H:306:SER:HB2	2.41	0.51
1:E:13:MSE:SE	1:E:329:VAL:HG22	2.60	0.51
1:H:86:LEU:HD23	1:I:317:ALA:HB2	1.93	0.51
1:G:328:ASP:O	1:G:332:ILE:HG13	2.10	0.51
1:D:94:LEU:HD21	1:D:98:SER:O	2.10	0.51
1:C:328:ASP:O	1:C:332:ILE:HG13	2.11	0.51
1:F:210:THR:N	1:F:211:PRO:CD	2.74	0.50
1:H:139:SER:O	1:H:143:GLN:HG2	2.10	0.50
1:A:281:GLN:NE2	1:F:67:ASN:HB2	2.26	0.50
1:E:328:ASP:O	1:E:332:ILE:HG13	2.12	0.50
1:I:65:TYR:OH	1:I:70:GLN:NE2	2.40	0.50
1:I:94:LEU:HD21	1:I:98:SER:O	2.11	0.50
1:D:94:LEU:HD23	1:D:94:LEU:C	2.36	0.50
1:A:13:MSE:SE	1:A:329:VAL:HG22	2.61	0.50
1:E:246[B]:GLN:OE1	1:F:152:LYS:HA	2.12	0.50
1:J:94:LEU:HD21	1:J:98:SER:O	2.12	0.50
1:C:257:ILE:HD11	1:D:147:VAL:HG11	1.94	0.50
1:E:260:GLN:CG	2:E:401:MPD:H52	2.28	0.50
1:F:20:ALA:HB2	1:F:282:MSE:HE1	1.94	0.50
1:H:210:THR:N	1:H:211:PRO:CD	2.75	0.50
1:C:210:THR:N	1:C:211:PRO:CD	2.75	0.50
1:E:257:ILE:HD11	1:F:147:VAL:HG11	1.93	0.50
1:J:94:LEU:C	1:J:94:LEU:HD23	2.36	0.50
1:E:210:THR:N	1:E:211:PRO:CD	2.75	0.50
1:E:238:LEU:HD13	1:F:247:LYS:CE	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:THR:N	1:D:211:PRO:CD	2.75	0.49
1:G:210:THR:N	1:G:211:PRO:CD	2.75	0.49
1:J:205:THR:OG1	1:J:207:GLY:O	2.23	0.49
1:J:210:THR:N	1:J:211:PRO:CD	2.74	0.49
1:G:281:GLN:OE1	1:I:67:ASN:ND2	2.34	0.49
1:B:210:THR:N	1:B:211:PRO:CD	2.75	0.49
1:D:32:GLN:HG3	1:E:271:GLN:OE1	2.13	0.49
1:F:94:LEU:C	1:F:94:LEU:HD23	2.37	0.49
1:J:125:ARG:NH1	1:J:283:SER:HB3	2.27	0.49
1:A:210:THR:N	1:A:211:PRO:CD	2.75	0.49
1:H:29:SER:OG	2:H:401:MPD:H13	2.13	0.49
1:I:210:THR:N	1:I:211:PRO:CD	2.75	0.49
1:B:94:LEU:C	1:B:94:LEU:HD23	2.38	0.48
1:G:86:LEU:HD23	1:J:317:ALA:HB2	1.96	0.48
1:I:115:THR:HA	1:I:297:ILE:HD11	1.95	0.48
1:F:149:LEU:HG	4:F:402:CL:CL	2.50	0.48
1:C:264:GLY:HA2	2:C:402:MPD:H32	1.96	0.48
1:F:115:THR:HA	1:F:297:ILE:HD11	1.94	0.48
1:C:13:MSE:N	1:C:282:MSE:HE1	2.26	0.48
1:E:107:LEU:HB2	1:E:297:ILE:CD1	2.44	0.48
1:E:238:LEU:HD12	1:F:247:LYS:HE3	1.95	0.47
1:G:90:ILE:HB	1:G:91:PRO:CD	2.44	0.47
1:J:185:GLY:HA3	2:J:402:MPD:HM2	1.96	0.47
1:F:94:LEU:HA	1:F:103:TRP:CZ3	2.50	0.47
1:G:336:ILE:HG22	1:J:284:ASN:HB3	1.96	0.47
1:B:205:THR:C	1:B:207:GLY:N	2.71	0.47
1:F:92:ALA:C	1:F:103:TRP:HH2	2.23	0.47
1:J:32:GLN:HG3	1:C:271:GLN:OE1	2.15	0.47
1:H:246:GLN:CD	1:I:43:ASN:HD21	2.23	0.47
1:A:90:ILE:HB	1:A:91:PRO:CD	2.44	0.47
4:C:404:CL:CL	1:D:43:ASN:HB2	2.51	0.47
1:E:238:LEU:CD1	1:F:247:LYS:CE	2.93	0.47
1:B:31:LYS:HE2	1:B:63:ASP:OD1	2.14	0.47
1:I:68:THR:C	1:I:71:PRO:HD2	2.40	0.47
1:F:210:THR:N	1:F:211:PRO:HD2	2.30	0.47
1:E:90:ILE:HB	1:E:91:PRO:CD	2.45	0.47
1:H:100:LYS:HE2	1:H:306:SER:HB2	1.97	0.47
1:J:306:SER:HB2	1:J:310:ILE:HG22	1.97	0.46
2:F:401:MPD:HM1	2:F:401:MPD:C5	2.46	0.46
1:J:68:THR:C	1:J:71:PRO:HD2	2.41	0.46
1:A:31:LYS:NZ	1:B:133:ASN:OD1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:ILE:HB	1:H:91:PRO:CD	2.46	0.46
1:G:204:VAL:O	1:G:205:THR:C	2.58	0.46
1:G:107:LEU:HB2	1:G:297:ILE:CD1	2.45	0.46
1:A:205:THR:HG23	1:A:208:THR:N	2.30	0.46
1:D:68:THR:C	1:D:71:PRO:HD2	2.41	0.46
1:B:68:THR:C	1:B:71:PRO:HD2	2.41	0.46
1:B:205:THR:O	1:B:205:THR:HG22	2.16	0.46
1:B:206:ALA:O	1:B:208:THR:N	2.48	0.46
1:C:204:VAL:O	1:C:205:THR:C	2.58	0.46
1:D:27:CYS:O	1:D:30:VAL:HG12	2.16	0.46
1:H:257:ILE:HD11	1:I:147:VAL:HG11	1.97	0.46
1:G:214:ILE:HG13	1:G:215:GLY:N	2.31	0.46
1:A:204:VAL:O	1:A:205:THR:C	2.58	0.46
1:B:115:THR:HA	1:B:297:ILE:HD11	1.98	0.46
1:E:68:THR:C	1:E:71:PRO:HD2	2.41	0.46
1:F:68:THR:C	1:F:71:PRO:HD2	2.41	0.46
1:H:107:LEU:HB2	1:H:297:ILE:CD1	2.45	0.46
1:G:104:LEU:HD23	1:G:300:LEU:HD23	1.98	0.46
1:G:271:GLN:OE1	1:I:32:GLN:HG3	2.16	0.46
1:J:27:CYS:O	1:J:30:VAL:HG12	2.16	0.46
1:C:90:ILE:HB	1:C:91:PRO:CD	2.45	0.46
1:D:115:THR:HA	1:D:297:ILE:HD11	1.97	0.46
1:I:125:ARG:HD2	1:I:287:ASP:OD1	2.16	0.46
1:I:324:THR:O	1:I:327:THR:OG1	2.26	0.46
1:J:197:ILE:CD1	1:C:214:ILE:HG12	2.46	0.45
1:A:68:THR:C	1:A:71:PRO:HD2	2.41	0.45
1:A:107:LEU:HB2	1:A:297:ILE:CD1	2.46	0.45
1:D:125:ARG:HD2	1:D:287:ASP:OD1	2.16	0.45
1:H:200:VAL:HG21	1:I:218:ALA:HA	1.98	0.45
1:J:115:THR:HA	1:J:297:ILE:HD11	1.97	0.45
1:A:257:ILE:HD11	1:B:147:VAL:HG11	1.98	0.45
1:B:306:SER:HB2	1:B:310:ILE:HG22	1.98	0.45
1:C:68:THR:C	1:C:71:PRO:HD2	2.42	0.45
1:G:68:THR:C	1:G:71:PRO:HD2	2.41	0.45
1:G:336:ILE:CG2	1:J:284:ASN:HB3	2.47	0.45
1:J:210:THR:N	1:J:211:PRO:HD2	2.32	0.45
1:J:257:ILE:HD12	1:J:257:ILE:HA	1.87	0.45
1:A:94:LEU:O	1:A:311:ARG:NH2	2.50	0.45
1:C:107:LEU:CB	1:C:297:ILE:CD1	2.95	0.45
2:F:401:MPD:HM1	2:F:401:MPD:H53	1.97	0.45
1:C:10:ASP:HB2	1:C:325:VAL:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ILE:HG13	1:E:314:TRP:HZ3	1.82	0.45
1:I:214:ILE:HG13	1:I:215:GLY:N	2.32	0.45
1:E:246[B]:GLN:NE2	1:F:156:ASP:OD1	2.50	0.45
1:F:94:LEU:HD21	1:F:98:SER:O	2.16	0.45
1:J:324:THR:O	1:J:327:THR:OG1	2.25	0.45
1:A:80:ILE:CD1	1:A:282:MSE:HE1	2.46	0.45
1:F:95:PRO:HD3	1:F:103:TRP:CZ3	2.52	0.45
1:J:67:ASN:HB3	1:C:281:GLN:CD	2.42	0.44
1:C:86:LEU:HD23	1:D:317:ALA:HB2	1.99	0.44
1:C:107:LEU:HB2	1:C:297:ILE:CD1	2.47	0.44
1:H:10:ASP:HB2	1:H:325:VAL:HG22	1.99	0.44
1:H:73:ILE:O	1:H:76:ASN:HB3	2.16	0.44
1:G:107:LEU:CB	1:G:297:ILE:CD1	2.96	0.44
1:D:257:ILE:HD12	1:D:257:ILE:HA	1.89	0.44
1:H:68:THR:C	1:H:71:PRO:HD2	2.42	0.44
1:H:94:LEU:O	1:H:311:ARG:NH2	2.50	0.44
1:G:36:VAL:HA	1:G:254:GLU:OE1	2.17	0.44
1:G:90:ILE:HB	1:G:91:PRO:HD3	2.00	0.44
1:G:90:ILE:HG13	1:G:314:TRP:HZ3	1.82	0.44
1:A:90:ILE:HG13	1:A:314:TRP:HZ3	1.81	0.44
1:B:70:GLN:N	1:B:71:PRO:CD	2.80	0.44
1:B:207:GLY:O	1:B:208:THR:HB	2.18	0.44
1:E:94:LEU:O	1:E:311:ARG:NH2	2.51	0.44
1:F:257:ILE:HD12	1:F:257:ILE:HA	1.88	0.44
1:G:94:LEU:O	1:G:311:ARG:NH2	2.51	0.44
1:B:27:CYS:O	1:B:30:VAL:HG12	2.17	0.44
1:C:90:ILE:HG13	1:C:314:TRP:HZ3	1.82	0.44
1:I:27:CYS:O	1:I:30:VAL:HG12	2.17	0.44
1:J:205:THR:C	1:J:207:GLY:N	2.75	0.44
1:A:107:LEU:CB	1:A:297:ILE:CD1	2.95	0.44
1:I:70:GLN:N	1:I:71:PRO:CD	2.81	0.44
1:E:196:ALA:CB	1:F:222:ALA:HA	2.47	0.44
1:E:13:MSE:HA	1:E:282:MSE:CE	2.48	0.44
1:E:107:LEU:HB2	1:E:297:ILE:HD11	2.00	0.43
1:F:27:CYS:O	1:F:30:VAL:HG12	2.18	0.43
1:D:70:GLN:N	1:D:71:PRO:CD	2.80	0.43
1:E:36:VAL:HA	1:E:254:GLU:OE1	2.18	0.43
1:J:70:GLN:N	1:J:71:PRO:CD	2.81	0.43
1:A:98:SER:HB2	1:A:102:GLN:OE1	2.19	0.43
1:B:32:GLN:HG3	1:H:271:GLN:OE1	2.19	0.43
1:H:107:LEU:CB	1:H:297:ILE:CD1	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:MSE:CA	1:C:282:MSE:HE1	2.43	0.43
1:F:36:VAL:HA	2:F:401:MPD:H12	2.01	0.43
1:B:302:LYS:HD2	1:B:314:TRP:CH2	2.54	0.43
1:G:246:GLN:HG3	1:J:43:ASN:HD21	1.84	0.43
1:C:36:VAL:HA	1:C:254:GLU:OE1	2.18	0.43
1:F:70:GLN:N	1:F:71:PRO:CD	2.81	0.43
1:F:91:PRO:HB2	1:F:103:TRP:CZ3	2.53	0.43
1:H:36:VAL:HA	1:H:254:GLU:OE1	2.18	0.43
1:A:36:VAL:HA	1:A:254:GLU:OE1	2.19	0.43
1:A:90:ILE:HB	1:A:91:PRO:HD3	2.00	0.43
1:E:10:ASP:HB2	1:E:325:VAL:HG22	2.01	0.43
1:D:181:ILE:HG21	2:E:402:MPD:CM	2.47	0.43
1:E:80:ILE:HD11	1:E:282:MSE:HE1	1.99	0.43
1:G:90:ILE:HD13	1:J:313:LEU:HD13	2.01	0.43
1:B:204:VAL:HG12	1:B:204:VAL:O	2.18	0.43
1:C:104:LEU:HD23	1:C:300:LEU:HD23	2.01	0.43
1:F:302:LYS:HD2	1:F:314:TRP:CH2	2.54	0.43
1:G:182:VAL:HG22	1:J:173:ALA:HB2	2.01	0.42
1:J:214:ILE:HG13	1:J:215:GLY:N	2.34	0.42
1:A:182:VAL:HG22	1:B:173:ALA:HB2	2.00	0.42
1:A:210:THR:N	1:A:211:PRO:HD2	2.34	0.42
1:H:70:GLN:N	1:H:71:PRO:CD	2.82	0.42
1:E:200:VAL:HG21	1:F:218:ALA:HA	2.01	0.42
1:G:90:ILE:HD12	1:G:106:GLN:HB3	2.01	0.42
1:J:186:LEU:HD13	1:C:187:LEU:HD11	2.01	0.42
1:C:15:ASN:ND2	1:C:281:GLN:NE2	2.45	0.42
1:H:282:MSE:HE3	1:H:286:TRP:NE1	2.35	0.42
1:G:70:GLN:N	1:G:71:PRO:CD	2.82	0.42
1:A:160:LEU:CD2	1:A:164:ASN:HD21	2.32	0.42
1:G:10:ASP:HB2	1:G:325:VAL:HG22	2.02	0.42
1:G:73:ILE:O	1:G:76:ASN:HB3	2.18	0.42
1:A:70:GLN:N	1:A:71:PRO:CD	2.83	0.42
1:E:70:GLN:N	1:E:71:PRO:CD	2.83	0.42
1:E:107:LEU:CB	1:E:297:ILE:CD1	2.96	0.42
1:J:197:ILE:HD12	1:C:214:ILE:HG12	2.01	0.42
1:E:90:ILE:HB	1:E:91:PRO:HD3	2.02	0.42
1:F:93:VAL:O	1:F:94:LEU:CB	2.67	0.42
1:F:242:GLN:O	1:F:246:GLN:HG3	2.20	0.42
1:A:271:GLN:OE1	1:F:32:GLN:HG3	2.20	0.42
1:C:70:GLN:N	1:C:71:PRO:CD	2.82	0.42
1:J:266:LYS:HA	1:J:266:LYS:HD3	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:VAL:HG22	1:H:270:VAL:HG21	2.02	0.42
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.87	0.42
1:G:193:PHE:CE1	1:J:226:GLY:HA3	2.55	0.42
1:D:214:ILE:HG13	1:D:215:GLY:N	2.35	0.42
1:E:80:ILE:CD1	1:E:282:MSE:HE1	2.50	0.42
1:B:242:GLN:O	1:B:246:GLN:HG3	2.20	0.41
1:H:90:ILE:HB	1:H:91:PRO:HD3	2.02	0.41
1:F:93:VAL:O	1:F:94:LEU:HB2	2.19	0.41
1:B:159:VAL:HG11	1:B:251:LEU:HD11	2.02	0.41
1:B:41:PHE:CD2	1:B:254:GLU:HB2	2.55	0.41
1:B:124:THR:HG21	1:B:286:TRP:CZ2	2.55	0.41
1:E:238:LEU:HD13	1:F:247:LYS:HD2	2.01	0.41
1:H:196:ALA:HB1	1:I:221:VAL:HG12	2.03	0.41
1:G:10:ASP:OD1	1:G:328:ASP:OD2	2.39	0.41
1:G:242:GLN:O	1:G:246:GLN:HG2	2.21	0.41
1:D:156:ASP:OD2	1:D:254:GLU:OE2	2.38	0.41
1:F:214:ILE:HG13	1:F:215:GLY:N	2.35	0.41
1:G:22:GLN:HB3	1:I:32:GLN:NE2	2.36	0.41
1:G:34:VAL:HA	1:G:35:PRO:HD3	1.94	0.41
1:D:242:GLN:O	1:D:246:GLN:HG3	2.21	0.41
1:H:86:LEU:O	1:H:87:GLN:C	2.64	0.41
1:I:242:GLN:O	1:I:246:GLN:HG3	2.21	0.41
1:C:173:ALA:HA	2:C:401:MPD:H32	2.03	0.41
2:C:401:MPD:O4	2:C:401:MPD:H11	2.21	0.41
1:E:58:ALA:HB2	1:E:265:TYR:CZ	2.56	0.41
1:F:95:PRO:CD	1:F:103:TRP:CE3	3.04	0.41
1:J:242:GLN:O	1:J:246:GLN:HG3	2.21	0.40
1:C:34:VAL:HA	1:C:35:PRO:HD3	1.95	0.40
1:C:210:THR:N	1:C:211:PRO:HD2	2.36	0.40
1:J:69:ILE:HG23	1:J:127:VAL:HG12	2.02	0.40
1:A:104:LEU:HD23	1:A:300:LEU:HD23	2.03	0.40
1:H:242:GLN:O	1:H:246:GLN:HG2	2.20	0.40
1:A:10:ASP:OD1	1:A:328:ASP:OD2	2.39	0.40
1:H:90:ILE:HG13	1:H:314:TRP:HZ3	1.84	0.40
1:H:104:LEU:HD23	1:H:300:LEU:HD23	2.02	0.40
1:A:73:ILE:O	1:A:76:ASN:HB3	2.22	0.40
1:A:95:PRO:O	1:A:98:SER:OG	2.38	0.40
1:B:254:GLU:O	1:B:257:ILE:HG22	2.22	0.40
1:C:90:ILE:HB	1:C:91:PRO:HD3	2.02	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	334/367 (91%)	323 (97%)	10 (3%)	1 (0%)	36	59
1	B	320/367 (87%)	307 (96%)	8 (2%)	5 (2%)	7	21
1	C	334/367 (91%)	323 (97%)	10 (3%)	1 (0%)	36	59
1	D	316/367 (86%)	307 (97%)	7 (2%)	2 (1%)	21	45
1	E	335/367 (91%)	325 (97%)	10 (3%)	0	100	100
1	F	313/367 (85%)	305 (97%)	6 (2%)	2 (1%)	21	45
1	G	334/367 (91%)	324 (97%)	9 (3%)	1 (0%)	36	59
1	H	333/367 (91%)	322 (97%)	11 (3%)	0	100	100
1	I	311/367 (85%)	303 (97%)	7 (2%)	1 (0%)	36	59
1	J	320/367 (87%)	307 (96%)	8 (2%)	5 (2%)	7	21
All	All	3250/3670 (89%)	3146 (97%)	86 (3%)	18 (1%)	21	45

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	205	THR
1	B	205	THR
1	B	207	GLY
1	B	208	THR
1	F	94	LEU
1	J	206	ALA
1	J	307	GLY
1	B	206	ALA
1	D	307	GLY
1	F	307	GLY
1	I	307	GLY
1	J	208	THR
1	B	307	GLY
1	G	204	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	204	VAL
1	J	204	VAL
1	C	204	VAL
1	D	204	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/288 (94%)	267 (98%)	5 (2%)	51	72
1	B	258/288 (90%)	255 (99%)	3 (1%)	63	78
1	C	272/288 (94%)	268 (98%)	4 (2%)	57	75
1	D	258/288 (90%)	255 (99%)	3 (1%)	63	78
1	E	272/288 (94%)	267 (98%)	5 (2%)	51	72
1	F	255/288 (88%)	250 (98%)	5 (2%)	48	70
1	G	272/288 (94%)	270 (99%)	2 (1%)	76	86
1	H	271/288 (94%)	268 (99%)	3 (1%)	65	80
1	I	253/288 (88%)	251 (99%)	2 (1%)	73	84
1	J	258/288 (90%)	252 (98%)	6 (2%)	44	68
All	All	2641/2880 (92%)	2603 (99%)	38 (1%)	59	76

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	99	THR
1	G	265	TYR
1	J	21	MSE
1	J	99	THR
1	J	100	LYS
1	J	210	THR
1	J	245	TYR
1	J	266	LYS
1	A	98	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	THR
1	A	148	ASN
1	A	265	TYR
1	A	282	MSE
1	B	21	MSE
1	B	99	THR
1	B	245	TYR
1	C	99	THR
1	C	148	ASN
1	C	265	TYR
1	C	282	MSE
1	D	21	MSE
1	D	99	THR
1	D	245	TYR
1	E	99	THR
1	E	148	ASN
1	E	203	PHE
1	E	265	TYR
1	E	282	MSE
1	F	21	MSE
1	F	99	THR
1	F	103	TRP
1	F	245	TYR
1	F	282	MSE
1	H	99	THR
1	H	148	ASN
1	H	265	TYR
1	I	21	MSE
1	I	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	15	ASN
1	G	16	GLN
1	G	76	ASN
1	G	82	ASN
1	G	87	GLN
1	G	162	GLN
1	G	269	GLN
1	J	70	GLN
1	J	79	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	162	GLN
1	J	246	GLN
1	J	271	GLN
1	A	16	GLN
1	A	87	GLN
1	A	281	GLN
1	B	70	GLN
1	C	11	GLN
1	C	15	ASN
1	C	16	GLN
1	C	40	GLN
1	C	76	ASN
1	C	82	ASN
1	C	87	GLN
1	C	246	GLN
1	C	269	GLN
1	D	16	GLN
1	D	43	ASN
1	D	70	GLN
1	D	72	GLN
1	D	113	GLN
1	D	148	ASN
1	D	271	GLN
1	D	284	ASN
1	E	11	GLN
1	E	15	ASN
1	E	16	GLN
1	E	82	ASN
1	E	87	GLN
1	E	260	GLN
1	E	269	GLN
1	F	61	HIS
1	F	162	GLN
1	F	236	ASN
1	F	246	GLN
1	F	284	ASN
1	H	3	ASN
1	H	11	GLN
1	H	15	ASN
1	H	16	GLN
1	H	82	ASN
1	H	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	260	GLN
1	H	269	GLN
1	I	43	ASN
1	I	61	HIS
1	I	70	GLN
1	I	72	GLN
1	I	82	ASN
1	I	162	GLN
1	I	271	GLN
1	I	284	ASN

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 53 ligands modelled in this entry, 37 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MPD	G	403	-	7,7,7	0.58	0	9,10,10	0.63	0
2	MPD	F	401	-	7,7,7	0.70	0	9,10,10	0.78	0
2	MPD	J	402	-	7,7,7	0.43	0	9,10,10	0.72	0
2	MPD	J	401	-	7,7,7	0.44	0	9,10,10	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	A	401	-	7,7,7	0.53	0	9,10,10	1.02	1 (11%)
2	MPD	G	401	-	7,7,7	0.52	0	9,10,10	1.36	2 (22%)
2	MPD	C	402	-	7,7,7	0.62	0	9,10,10	0.65	0
2	MPD	E	402	-	7,7,7	0.62	0	9,10,10	1.80	2 (22%)
2	MPD	C	401	-	7,7,7	0.49	0	9,10,10	1.01	1 (11%)
2	MPD	E	401	-	7,7,7	0.55	0	9,10,10	1.11	0
2	MPD	H	402	-	7,7,7	0.49	0	9,10,10	0.57	0
2	MPD	G	402	-	7,7,7	0.51	0	9,10,10	0.67	0
2	MPD	I	401	-	7,7,7	0.80	0	9,10,10	1.19	1 (11%)
3	PO4	E	403	-	4,4,4	0.99	0	6,6,6	0.62	0
2	MPD	H	401	-	7,7,7	0.38	0	9,10,10	0.61	0
3	PO4	G	404	-	4,4,4	0.94	0	6,6,6	0.87	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
2	MPD	G	403	-	-	2/5/5/5	-
2	MPD	F	401	-	-	2/5/5/5	-
2	MPD	J	402	-	-	2/5/5/5	-
2	MPD	J	401	-	-	2/5/5/5	-
2	MPD	A	401	-	-	1/5/5/5	-
2	MPD	G	401	-	-	0/5/5/5	-
2	MPD	C	402	-	-	2/5/5/5	-
2	MPD	E	402	-	-	1/5/5/5	-
2	MPD	C	401	-	-	2/5/5/5	-
2	MPD	E	401	-	-	2/5/5/5	-
2	MPD	H	402	-	-	0/5/5/5	-
2	MPD	G	402	-	-	3/5/5/5	-
2	MPD	I	401	-	-	1/5/5/5	-
2	MPD	H	401	-	-	1/5/5/5	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	402	MPD	CM-C2-C1	-3.23	103.40	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	MPD	CM-C2-C1	2.65	116.55	110.63
2	A	401	MPD	O2-C2-C3	-2.23	100.94	109.27
2	I	401	MPD	O2-C2-CM	-2.10	101.44	107.99
2	G	401	MPD	O2-C2-C1	-2.07	101.55	107.99
2	E	402	MPD	O2-C2-C1	2.03	114.32	107.99
2	C	401	MPD	O4-C4-C3	-2.03	103.29	111.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	402	MPD	C1-C2-C3-C4
2	G	402	MPD	O2-C2-C3-C4
2	C	402	MPD	C2-C3-C4-C5
2	E	402	MPD	C2-C3-C4-C5
2	F	401	MPD	C2-C3-C4-O4
2	F	401	MPD	C2-C3-C4-C5
2	A	401	MPD	O2-C2-C3-C4
2	G	403	MPD	C2-C3-C4-O4
2	G	402	MPD	CM-C2-C3-C4
2	G	403	MPD	C2-C3-C4-C5
2	J	402	MPD	O2-C2-C3-C4
2	C	401	MPD	O2-C2-C3-C4
2	E	401	MPD	O2-C2-C3-C4
2	H	401	MPD	O2-C2-C3-C4
2	I	401	MPD	O2-C2-C3-C4
2	J	401	MPD	C1-C2-C3-C4
2	J	401	MPD	CM-C2-C3-C4
2	J	402	MPD	C1-C2-C3-C4
2	C	401	MPD	C1-C2-C3-C4
2	C	402	MPD	C1-C2-C3-C4
2	E	401	MPD	C1-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	MPD	3	0
2	J	402	MPD	1	0
2	C	402	MPD	1	0
2	E	402	MPD	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	MPD	2	0
2	E	401	MPD	2	0
2	H	401	MPD	3	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	332/367 (90%)	0.45	22 (6%) 24 21	47, 70, 120, 139	0
1	B	318/367 (86%)	0.39	29 (9%) 15 13	44, 67, 119, 160	0
1	C	332/367 (90%)	0.37	23 (6%) 23 19	31, 61, 111, 141	0
1	D	316/367 (86%)	0.15	23 (7%) 21 18	38, 56, 113, 158	0
1	E	332/367 (90%)	0.36	22 (6%) 24 21	30, 66, 122, 156	1 (0%)
1	F	313/367 (85%)	0.34	28 (8%) 15 14	39, 67, 117, 142	0
1	G	332/367 (90%)	0.23	19 (5%) 29 24	35, 62, 108, 156	0
1	H	331/367 (90%)	0.51	22 (6%) 24 21	46, 74, 126, 150	0
1	I	311/367 (84%)	0.29	18 (5%) 29 23	42, 66, 119, 151	0
1	J	318/367 (86%)	0.12	14 (4%) 39 31	35, 54, 101, 149	0
All	All	3235/3670 (88%)	0.32	220 (6%) 23 20	30, 65, 119, 160	1 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	VAL	6.3
1	J	203	PHE	5.2
1	F	208	THR	5.0
1	H	302	LYS	4.9
1	A	235	HIS	4.9
1	J	208	THR	4.6
1	G	302	LYS	4.6
1	B	200	VAL	4.5
1	C	235	HIS	4.4
1	E	200	VAL	4.3
1	H	205	THR	4.3
1	I	200	VAL	4.2
1	F	210	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	214	ILE	4.2
1	C	2	THR	4.1
1	B	199	ALA	4.0
1	D	204	VAL	3.9
1	C	208	THR	3.9
1	B	337	ALA	3.9
1	J	212	VAL	3.8
1	E	235	HIS	3.8
1	B	203	PHE	3.8
1	E	302	LYS	3.8
1	E	341	PRO	3.7
1	H	341	PRO	3.7
1	H	235	HIS	3.7
1	B	198	GLY	3.6
1	D	200	VAL	3.6
1	C	100	LYS	3.6
1	H	209	SER	3.5
1	G	2	THR	3.5
1	I	201	ALA	3.5
1	J	214	ILE	3.5
1	C	203	PHE	3.5
1	A	208	THR	3.5
1	A	203	PHE	3.4
1	F	304	ILE	3.4
1	E	203	PHE	3.4
1	A	341	PRO	3.4
1	C	56	ASP	3.3
1	F	203	PHE	3.3
1	D	213	VAL	3.3
1	B	243	ASP	3.3
1	J	211	PRO	3.3
1	B	204	VAL	3.3
1	B	112	GLU	3.2
1	H	203	PHE	3.2
1	I	212	VAL	3.2
1	C	238	LEU	3.2
1	F	245	TYR	3.1
1	E	100	LYS	3.1
1	F	199	ALA	3.1
1	H	200	VAL	3.1
1	B	214	ILE	3.1
1	D	243	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	301	ASP	3.1
1	I	214	ILE	3.1
1	D	203	PHE	3.1
1	J	206	ALA	3.0
1	C	302	LYS	3.0
1	G	208	THR	3.0
1	B	301	ASP	3.0
1	F	214	ILE	3.0
1	A	319	ASP	3.0
1	F	309	ASP	2.9
1	A	2	THR	2.9
1	H	2	THR	2.9
1	A	100	LYS	2.9
1	E	157	ASN	2.9
1	B	213	VAL	2.9
1	H	101	ALA	2.9
1	J	210	THR	2.9
1	F	91	PRO	2.8
1	F	100	LYS	2.8
1	G	204	VAL	2.8
1	C	319	ASP	2.8
1	C	237	SER	2.8
1	D	205	THR	2.8
1	F	103	TRP	2.8
1	J	200	VAL	2.8
1	C	307	GLY	2.8
1	D	212	VAL	2.7
1	D	199	ALA	2.7
1	I	92	ALA	2.7
1	I	247	LYS	2.7
1	H	157	ASN	2.7
1	C	308	ASP	2.7
1	H	211	PRO	2.7
1	G	237	SER	2.7
1	F	92	ALA	2.7
1	A	205	THR	2.7
1	H	199	ALA	2.7
1	D	15	ASN	2.7
1	D	198	GLY	2.7
1	A	304	ILE	2.6
1	H	304	ILE	2.6
1	D	211	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	205	THR	2.6
1	E	2	THR	2.6
1	A	204	VAL	2.6
1	D	202	ASP	2.6
1	I	16	GLN	2.6
1	G	199	ALA	2.6
1	I	209	SER	2.6
1	G	341	PRO	2.6
1	B	210	THR	2.6
1	H	335	GLN	2.6
1	C	239	GLY	2.6
1	H	238	LEU	2.5
1	B	197	ILE	2.5
1	B	212	VAL	2.5
1	A	157	ASN	2.5
1	A	302	LYS	2.5
1	I	100	LYS	2.5
1	C	211	PRO	2.5
1	F	306	SER	2.5
1	F	310	ILE	2.5
1	B	206	ALA	2.5
1	E	305	THR	2.5
1	B	211	PRO	2.4
1	G	203	PHE	2.4
1	H	100	LYS	2.4
1	B	86	LEU	2.4
1	D	195	THR	2.4
1	E	99	THR	2.4
1	F	95	PRO	2.4
1	G	148	ASN	2.4
1	F	202	ASP	2.4
1	F	209	SER	2.4
1	A	238	LEU	2.4
1	C	341	PRO	2.4
1	B	16	GLN	2.3
1	B	116	GLU	2.3
1	E	199	ALA	2.3
1	F	101	ALA	2.3
1	B	247	LYS	2.3
1	F	200	VAL	2.3
1	A	239	GLY	2.3
1	C	335	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	86	LEU	2.3
1	E	204	VAL	2.3
1	I	109	VAL	2.3
1	E	106	GLN	2.3
1	B	209	SER	2.3
1	B	307	GLY	2.3
1	G	335	GLN	2.2
1	H	212	VAL	2.2
1	A	335	GLN	2.2
1	A	105	ARG	2.2
1	A	211	PRO	2.2
1	B	108	SER	2.2
1	I	310	ILE	2.2
1	I	309	ASP	2.2
1	D	217	VAL	2.2
1	F	109	VAL	2.2
1	B	208	THR	2.2
1	F	86	LEU	2.2
1	A	112	GLU	2.2
1	E	105	ARG	2.2
1	J	16	GLN	2.2
1	F	67	ASN	2.2
1	D	210	THR	2.2
1	J	307	GLY	2.2
1	E	256	LEU	2.2
1	G	201	ALA	2.2
1	G	200	VAL	2.1
1	F	93	VAL	2.1
1	I	91	PRO	2.1
1	A	198	GLY	2.1
1	E	208	THR	2.1
1	H	305	THR	2.1
1	J	245	TYR	2.1
1	C	101	ALA	2.1
1	J	105	ARG	2.1
1	G	3	ASN	2.1
1	C	212	VAL	2.1
1	D	247	LYS	2.1
1	G	301	ASP	2.1
1	B	299	ASP	2.1
1	B	215	GLY	2.1
1	D	307	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	198	GLY	2.1
1	C	105	ARG	2.1
1	E	197	ILE	2.1
1	E	304	ILE	2.1
1	I	304	ILE	2.1
1	G	212	VAL	2.1
1	A	200	VAL	2.1
1	J	168	ASP	2.1
1	J	243	ASP	2.1
1	E	307	GLY	2.1
1	B	205	THR	2.1
1	A	197	ILE	2.1
1	B	196	ALA	2.1
1	C	232	ILE	2.1
1	G	235	HIS	2.1
1	F	302	LYS	2.1
1	C	157	ASN	2.1
1	E	207	GLY	2.1
1	H	99	THR	2.1
1	I	308	ASP	2.1
1	D	196	ALA	2.1
1	D	197	ILE	2.1
1	C	234	LEU	2.0
1	B	226	GLY	2.0
1	E	239	GLY	2.0
1	F	307	GLY	2.0
1	D	201	ALA	2.0
1	H	56	ASP	2.0
1	H	309	ASP	2.0
1	F	108	SER	2.0
1	E	96	PRO	2.0
1	H	315	LEU	2.0
1	G	157	ASN	2.0
1	I	197	ILE	2.0
1	A	101	ALA	2.0
1	F	337	ALA	2.0
1	G	56	ASP	2.0
1	D	45	LYS	2.0
1	F	212	VAL	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($\text{\AA}^2$)	Q<0.9
4	CL	C	404	1/1	0.68	0.21	118,118,118,118	0
5	NA	C	409	1/1	0.70	0.41	83,83,83,83	0
3	PO4	G	404	5/5	0.81	0.26	134,155,173,200	0
5	NA	B	403	1/1	0.89	0.21	92,92,92,92	0
2	MPD	F	401	8/8	0.89	0.20	62,76,84,84	0
4	CL	E	405	1/1	0.90	0.21	78,78,78,78	0
5	NA	E	406	1/1	0.90	0.36	65,65,65,65	0
2	MPD	E	402	8/8	0.91	0.20	70,77,86,92	0
4	CL	H	405	1/1	0.91	0.16	75,75,75,75	0
3	PO4	E	403	5/5	0.91	0.12	113,127,132,139	0
4	CL	G	405	1/1	0.91	0.17	87,87,87,87	0
2	MPD	I	401	8/8	0.91	0.20	62,76,85,89	0
4	CL	A	402	1/1	0.92	0.14	107,107,107,107	0
4	CL	F	403	1/1	0.92	0.10	76,76,76,76	0
4	CL	I	402	1/1	0.93	0.28	82,82,82,82	0
2	MPD	G	403	8/8	0.93	0.20	79,82,98,100	0
4	CL	H	403	1/1	0.93	0.14	98,98,98,98	0
4	CL	C	403	1/1	0.93	0.09	68,68,68,68	0
4	CL	B	401	1/1	0.94	0.15	69,69,69,69	0
4	CL	B	402	1/1	0.94	0.31	102,102,102,102	0
2	MPD	G	401	8/8	0.94	0.16	68,74,77,77	0
2	MPD	A	401	8/8	0.94	0.17	74,82,91,92	0
4	CL	I	405	1/1	0.94	0.10	76,76,76,76	0
4	CL	C	405	1/1	0.94	0.11	83,83,83,83	0
2	MPD	G	402	8/8	0.94	0.15	76,80,84,85	0
4	CL	F	402	1/1	0.94	0.26	92,92,92,92	0
5	NA	E	407	1/1	0.94	0.15	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	H	402	8/8	0.95	0.17	85,96,99,100	0
4	CL	F	404	1/1	0.95	0.11	72,72,72,72	0
4	CL	F	405	1/1	0.95	0.17	72,72,72,72	0
2	MPD	C	402	8/8	0.95	0.16	50,63,66,70	0
2	MPD	E	401	8/8	0.95	0.15	63,72,78,78	0
2	MPD	J	401	8/8	0.95	0.19	66,75,77,79	0
2	MPD	C	401	8/8	0.95	0.17	64,71,73,76	0
4	CL	C	407	1/1	0.95	0.17	84,84,84,84	0
4	CL	E	404	1/1	0.95	0.13	82,82,82,82	0
5	NA	C	410	1/1	0.95	0.33	60,60,60,60	0
4	CL	G	406	1/1	0.95	0.08	61,61,61,61	0
2	MPD	H	401	8/8	0.95	0.15	67,80,82,90	0
2	MPD	J	402	8/8	0.96	0.16	87,92,103,104	0
5	NA	D	403	1/1	0.96	0.39	60,60,60,60	0
4	CL	H	404	1/1	0.96	0.18	68,68,68,68	0
4	CL	I	404	1/1	0.96	0.15	83,83,83,83	0
5	NA	H	406	1/1	0.96	0.13	63,63,63,63	0
4	CL	D	401	1/1	0.97	0.28	94,94,94,94	0
5	NA	J	404	1/1	0.97	0.18	62,62,62,62	0
5	NA	F	406	1/1	0.97	0.27	60,60,60,60	0
4	CL	C	406	1/1	0.97	0.13	62,62,62,62	0
4	CL	J	403	1/1	0.98	0.36	90,90,90,90	0
4	CL	I	403	1/1	0.98	0.09	63,63,63,63	0
5	NA	C	408	1/1	0.98	0.08	39,39,39,39	0
4	CL	G	407	1/1	0.98	0.20	64,64,64,64	0
4	CL	D	402	1/1	0.98	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.