



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:30 AM GMT

PDB ID : 1R3N
Title : Crystal structure of beta-alanine synthase from *Saccharomyces kluyveri*
Authors : Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritsch, D.
Deposited on : 2003-10-02
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

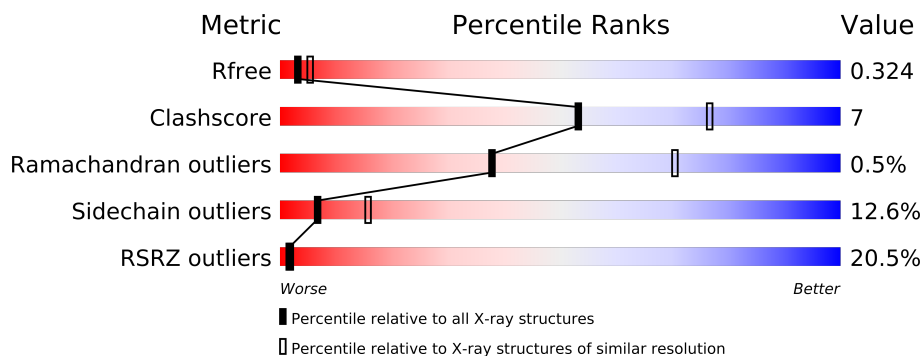
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	462	
1	B	462	
1	C	462	
1	D	462	
1	E	462	
1	F	462	
1	G	462	
1	H	462	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	BIB	C	3502	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	BIB	E	6502	-	X
3	BIB	G	8502	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27487 atoms, of which 0 are hydrogen and 0 are deuterium.

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 beta-alanine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	B	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	C	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	D	437	Total	C	N	O	S	0	0	0
			3375	2128	579	652	16			
1	E	433	Total	C	N	O	S	0	0	0
			3344	2108	574	646	16			
1	F	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			
1	G	430	Total	C	N	O	S	0	0	0
			3327	2097	571	643	16			
1	H	438	Total	C	N	O	S	0	0	0
			3379	2130	580	653	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	HIS	-	EXPRESSION TAG	UNP Q96W94
A	457	HIS	-	EXPRESSION TAG	UNP Q96W94
A	458	HIS	-	EXPRESSION TAG	UNP Q96W94
A	459	HIS	-	EXPRESSION TAG	UNP Q96W94
A	460	HIS	-	EXPRESSION TAG	UNP Q96W94
A	461	HIS	-	EXPRESSION TAG	UNP Q96W94
A	462	HIS	-	EXPRESSION TAG	UNP Q96W94
A	463	HIS	-	EXPRESSION TAG	UNP Q96W94
B	456	HIS	-	EXPRESSION TAG	UNP Q96W94
B	457	HIS	-	EXPRESSION TAG	UNP Q96W94
B	458	HIS	-	EXPRESSION TAG	UNP Q96W94
B	459	HIS	-	EXPRESSION TAG	UNP Q96W94
B	460	HIS	-	EXPRESSION TAG	UNP Q96W94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	EXPRESSION TAG	UNP Q96W94
B	462	HIS	-	EXPRESSION TAG	UNP Q96W94
B	463	HIS	-	EXPRESSION TAG	UNP Q96W94
C	456	HIS	-	EXPRESSION TAG	UNP Q96W94
C	457	HIS	-	EXPRESSION TAG	UNP Q96W94
C	458	HIS	-	EXPRESSION TAG	UNP Q96W94
C	459	HIS	-	EXPRESSION TAG	UNP Q96W94
C	460	HIS	-	EXPRESSION TAG	UNP Q96W94
C	461	HIS	-	EXPRESSION TAG	UNP Q96W94
C	462	HIS	-	EXPRESSION TAG	UNP Q96W94
C	463	HIS	-	EXPRESSION TAG	UNP Q96W94
D	456	HIS	-	EXPRESSION TAG	UNP Q96W94
D	457	HIS	-	EXPRESSION TAG	UNP Q96W94
D	458	HIS	-	EXPRESSION TAG	UNP Q96W94
D	459	HIS	-	EXPRESSION TAG	UNP Q96W94
D	460	HIS	-	EXPRESSION TAG	UNP Q96W94
D	461	HIS	-	EXPRESSION TAG	UNP Q96W94
D	462	HIS	-	EXPRESSION TAG	UNP Q96W94
D	463	HIS	-	EXPRESSION TAG	UNP Q96W94
E	456	HIS	-	EXPRESSION TAG	UNP Q96W94
E	457	HIS	-	EXPRESSION TAG	UNP Q96W94
E	458	HIS	-	EXPRESSION TAG	UNP Q96W94
E	459	HIS	-	EXPRESSION TAG	UNP Q96W94
E	460	HIS	-	EXPRESSION TAG	UNP Q96W94
E	461	HIS	-	EXPRESSION TAG	UNP Q96W94
E	462	HIS	-	EXPRESSION TAG	UNP Q96W94
E	463	HIS	-	EXPRESSION TAG	UNP Q96W94
F	456	HIS	-	EXPRESSION TAG	UNP Q96W94
F	457	HIS	-	EXPRESSION TAG	UNP Q96W94
F	458	HIS	-	EXPRESSION TAG	UNP Q96W94
F	459	HIS	-	EXPRESSION TAG	UNP Q96W94
F	460	HIS	-	EXPRESSION TAG	UNP Q96W94
F	461	HIS	-	EXPRESSION TAG	UNP Q96W94
F	462	HIS	-	EXPRESSION TAG	UNP Q96W94
F	463	HIS	-	EXPRESSION TAG	UNP Q96W94
G	456	HIS	-	EXPRESSION TAG	UNP Q96W94
G	457	HIS	-	EXPRESSION TAG	UNP Q96W94
G	458	HIS	-	EXPRESSION TAG	UNP Q96W94
G	459	HIS	-	EXPRESSION TAG	UNP Q96W94
G	460	HIS	-	EXPRESSION TAG	UNP Q96W94
G	461	HIS	-	EXPRESSION TAG	UNP Q96W94
G	462	HIS	-	EXPRESSION TAG	UNP Q96W94

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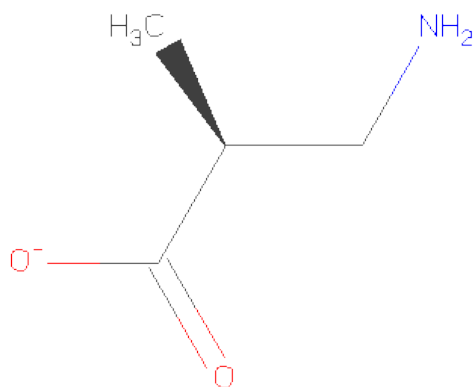
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Chain	Residue	Modelled	Actual	Comment	Reference
G	463	HIS	-	EXPRESSION TAG	UNP Q96W94
H	456	HIS	-	EXPRESSION TAG	UNP Q96W94
H	457	HIS	-	EXPRESSION TAG	UNP Q96W94
H	458	HIS	-	EXPRESSION TAG	UNP Q96W94
H	459	HIS	-	EXPRESSION TAG	UNP Q96W94
H	460	HIS	-	EXPRESSION TAG	UNP Q96W94
H	461	HIS	-	EXPRESSION TAG	UNP Q96W94
H	462	HIS	-	EXPRESSION TAG	UNP Q96W94
H	463	HIS	-	EXPRESSION TAG	UNP Q96W94

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: C₄H₈NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	4	1	2		
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		
3	D	1	Total	C	N	O	0	0
			7	4	1	2		
3	E	1	Total	C	N	O	0	0
			7	4	1	2		
3	E	1	Total	C	N	O	0	0
			7	4	1	2		
3	G	1	Total	C	N	O	0	0
			7	4	1	2		
3	G	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	60	Total	O	0	0
			60	60		
4	C	91	Total	O	0	0
			91	91		
4	D	54	Total	O	0	0
			54	54		

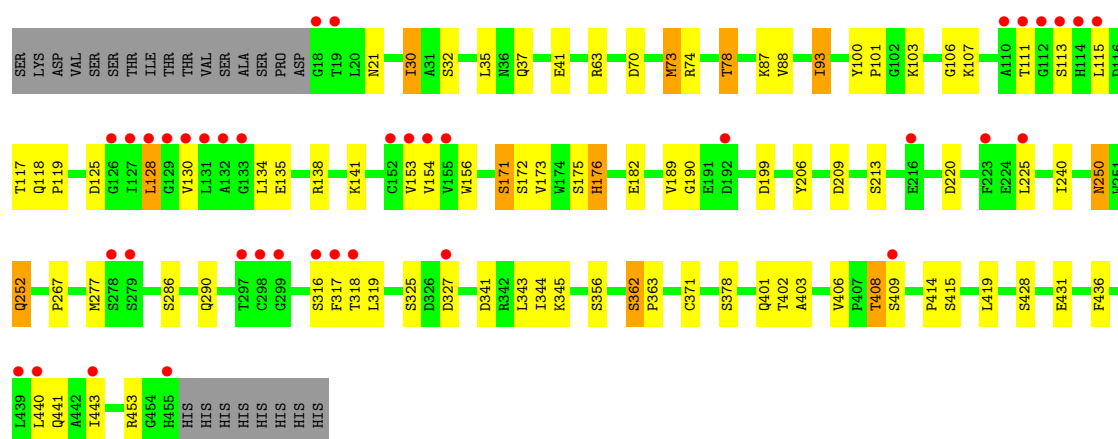
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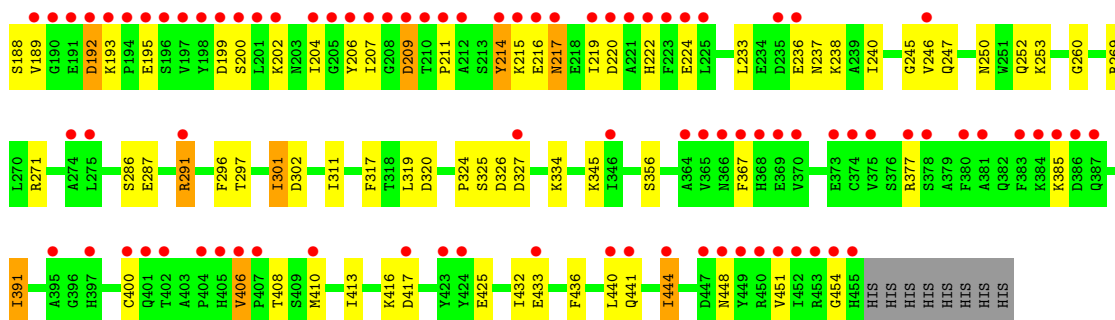
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	20	Total 20	O 20	0	0
4	F	101	Total 101	O 101	0	0
4	G	24	Total 24	O 24	0	0
4	H	50	Total 50	O 50	0	0

- Molecule 1: beta-alanine synthase

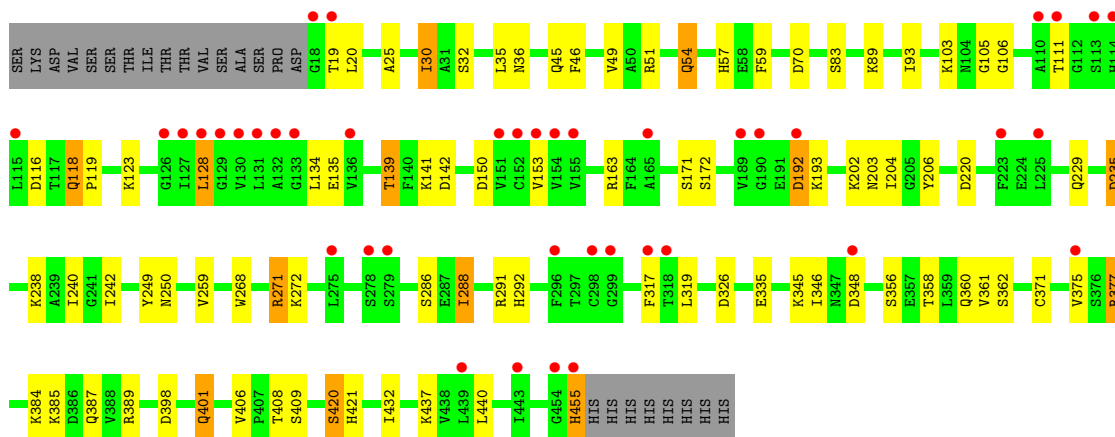
Chain C:





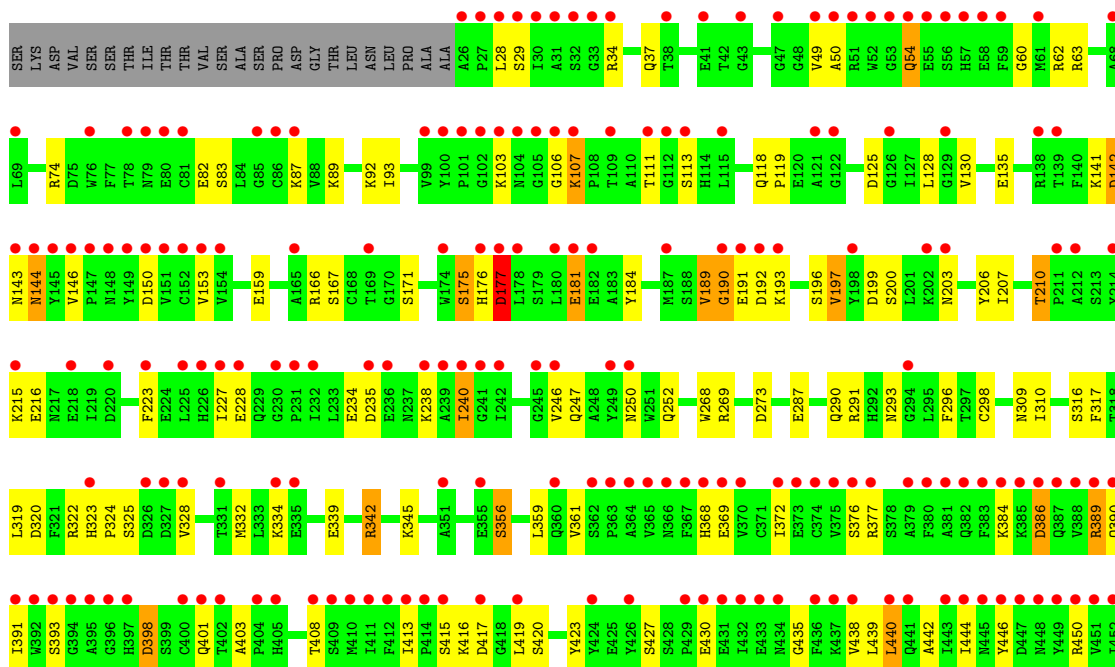
• Molecule 1: beta-alanine synthase

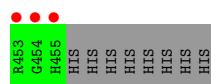
Chain F: 



• Molecule 1: beta-alanine synthase

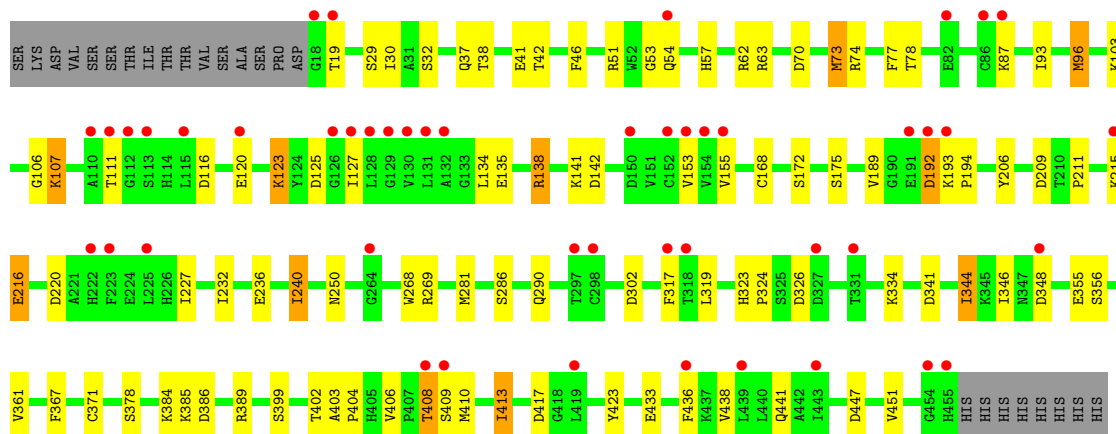
Chain G: 





- Molecule 1: beta-alanine synthase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.23Å 77.12Å 225.52Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 24.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-2.70) 95.9 (24.90-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.266 0.292 , 0.324	Depositor DCC
R_{free} test set	5290 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	10 of 106175 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27487	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.92 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.5506e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	1/3457 (0.0%)	0.80	15/4689 (0.3%)
1	B	0.43	0/3422	0.75	14/4640 (0.3%)
1	C	0.52	0/3457	0.75	6/4689 (0.1%)
1	D	0.44	0/3453	0.73	8/4684 (0.2%)
1	E	0.39	0/3422	0.71	10/4640 (0.2%)
1	F	0.49	0/3457	0.73	7/4689 (0.1%)
1	G	0.38	0/3404	0.72	13/4615 (0.3%)
1	H	0.44	0/3457	0.74	12/4689 (0.3%)
All	All	0.46	1/27529 (0.0%)	0.74	85/37335 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLY	C-O	-9.59	1.08	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	125	ASP	CB-CG-OD2	9.55	126.90	118.30
1	B	125	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	105	GLY	CA-C-N	8.52	133.25	116.20
1	D	125	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	309	ASN	CB-CA-C	-7.89	94.61	110.40
1	H	209	ASP	CB-CG-OD2	7.17	124.75	118.30
1	G	125	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	327	ASP	CB-CG-OD2	6.89	124.50	118.30
1	G	309	ASN	CB-CA-C	-6.83	96.73	110.40
1	B	142	ASP	CB-CG-OD2	6.76	124.39	118.30
1	C	125	ASP	CB-CG-OD2	6.65	124.28	118.30
1	B	319	LEU	CA-CB-CG	6.53	130.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	235	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	116	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	320	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	348	ASP	CB-CG-OD2	6.35	124.01	118.30
1	F	116	ASP	CB-CG-OD2	6.20	123.88	118.30
1	F	235	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	75	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	105	GLY	CA-C-O	-6.04	109.72	120.60
1	B	177	ASP	CB-CG-OD2	6.03	123.72	118.30
1	G	150	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	220	ASP	CB-CG-OD2	6.00	123.70	118.30
1	F	70	ASP	CB-CG-OD2	6.00	123.70	118.30
1	H	326	ASP	CB-CG-OD2	5.97	123.68	118.30
1	H	341	ASP	CB-CG-OD2	5.91	123.61	118.30
1	G	177	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	309	ASN	N-CA-CB	-5.86	100.05	110.60
1	H	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	150	ASP	CB-CG-OD2	5.77	123.49	118.30
1	G	273	ASP	CB-CG-OD2	5.75	123.48	118.30
1	E	302	ASP	CB-CG-OD2	5.74	123.47	118.30
1	G	440	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	320	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	192	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	220	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	386	ASP	CB-CG-OD2	5.63	123.37	118.30
1	F	142	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	302	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	209	ASP	CB-CG-OD2	5.58	123.32	118.30
1	F	326	ASP	CB-CG-OD2	5.55	123.30	118.30
1	G	386	ASP	CB-CG-OD2	5.53	123.27	118.30
1	H	386	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	447	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	199	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	220	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	70	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	70	ASP	CB-CG-OD2	5.47	123.23	118.30
1	F	220	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	320	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	192	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	220	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	116	ASP	CB-CG-OD2	5.35	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	142	ASP	CB-CG-OD2	5.35	123.12	118.30
1	G	320	ASP	CB-CG-OD2	5.34	123.11	118.30
1	G	417	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	447	ASP	CB-CG-OD2	5.32	123.09	118.30
1	G	192	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	150	ASP	CB-CG-OD2	5.32	123.08	118.30
1	E	326	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	105	GLY	N-CA-C	5.30	126.35	113.10
1	E	177	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	192	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	22	LEU	CA-CB-CG	5.26	127.40	115.30
1	E	320	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	348	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	327	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	125	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	209	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	199	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	220	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	199	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	341	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	417	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	327	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	150	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	177	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	70	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	209	ASP	CB-CG-OD2	5.06	122.85	118.30
1	G	235	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	398	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	150	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	199	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	341	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3379	0	3264	49	0
1	B	3344	0	3227	39	1
1	C	3379	0	3264	44	0
1	D	3375	0	3261	39	0
1	E	3344	0	3227	73	0
1	F	3379	0	3264	41	0
1	G	3327	0	3209	51	1
1	H	3379	0	3264	44	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
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	7	0	8	1	0
3	B	7	0	8	0	0
3	C	7	0	8	0	0
3	D	7	0	8	0	0
3	E	14	0	16	0	0
3	G	14	0	16	0	0
4	A	109	0	0	4	0
4	B	60	0	0	3	0
4	C	91	0	0	2	0
4	D	54	0	0	3	0
4	E	20	0	0	0	0
4	F	101	0	0	3	0
4	G	24	0	0	3	0
4	H	50	0	0	2	0
All	All	27487	0	26044	370	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (370) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:189:VAL:HG23	1:D:190:GLY:H	1.24	1.03
1:E:118:GLN:HG3	1:E:119:PRO:HD2	1.47	0.96
1:E:71:GLY:HA3	1:E:204:ILE:CG2	1.97	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:346:ILE:HD11	4:H:511:HOH:O	1.68	0.93
1:B:55:GLU:HB2	1:B:58:GLU:HG3	1.49	0.90
1:E:78:THR:HG23	1:E:88:VAL:HG11	1.54	0.89
1:E:211:PRO:O	1:E:217:ASN:ND2	2.06	0.89
1:C:189:VAL:HG23	1:C:190:GLY:H	1.40	0.86
1:F:135:GLU:O	1:F:139:THR:HG23	1.78	0.82
1:E:247:GLN:HE21	1:E:324:PRO:HD3	1.46	0.81
1:C:118:GLN:HG3	1:C:119:PRO:HD2	1.63	0.81
1:E:135:GLU:O	1:E:139:THR:HG23	1.80	0.80
1:B:371:CYS:HB3	1:B:409:SER:HB3	1.63	0.79
1:F:118:GLN:HG3	1:F:119:PRO:CD	2.12	0.78
1:E:448:ASN:O	1:E:451:VAL:HG12	1.84	0.78
1:D:296:PHE:CE1	1:D:319:LEU:HD23	2.19	0.78
1:E:30:ILE:CG2	1:E:436:PHE:HE2	1.96	0.78
1:H:74:ARG:O	1:H:78:THR:HG23	1.84	0.77
1:E:71:GLY:HA3	1:E:204:ILE:HG21	1.64	0.77
1:A:309:ASN:HD21	3:A:2502:BIB:H3	1.50	0.77
1:B:112:GLY:HA3	1:B:154:VAL:HG22	1.65	0.76
1:C:37:GLN:O	1:C:41:GLU:HG3	1.86	0.75
1:E:71:GLY:CA	1:E:204:ILE:HG21	2.17	0.74
1:D:413:ILE:HD11	1:D:435:GLY:CA	2.19	0.73
1:E:71:GLY:HA3	1:E:204:ILE:HG23	1.69	0.72
1:C:74:ARG:O	1:C:78:THR:HG22	1.90	0.72
1:D:296:PHE:HE1	1:D:319:LEU:HD23	1.52	0.72
1:D:189:VAL:HG23	1:D:190:GLY:N	2.02	0.72
1:H:62:ARG:HD2	4:H:538:HOH:O	1.90	0.72
1:F:455:HIS:CD2	1:F:455:HIS:N	2.58	0.71
1:C:317:PHE:CE1	1:C:319:LEU:HD21	2.25	0.70
1:G:89:LYS:HB3	1:G:210:THR:HG21	1.74	0.70
1:E:236:GLU:O	1:E:238:LYS:HE3	1.91	0.70
1:C:118:GLN:HG3	1:C:119:PRO:CD	2.22	0.70
1:C:371:CYS:HB3	1:C:409:SER:HB2	1.74	0.69
1:E:53:GLY:HA3	1:E:58:GLU:OE1	1.92	0.69
1:A:74:ARG:O	1:A:78:THR:HG22	1.92	0.69
1:C:63:ARG:CZ	1:C:73:MET:HG3	2.23	0.69
1:E:96:MET:SD	1:E:206:TYR:HE2	2.16	0.68
1:F:118:GLN:HG3	1:F:119:PRO:HD2	1.74	0.68
1:H:317:PHE:CE1	1:H:319:LEU:HD21	2.28	0.68
1:D:247:GLN:HE21	1:D:324:PRO:HD3	1.58	0.68
1:D:189:VAL:CG2	1:D:190:GLY:H	2.06	0.67
1:A:371:CYS:HB3	1:A:409:SER:HB2	1.77	0.67
1:E:269:ARG:NH2	1:F:235:ASP:OD1	2.26	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:GLU:OE2	4:A:2567:HOH:O	2.11	0.67
1:C:189:VAL:HG23	1:C:190:GLY:N	2.07	0.66
1:D:244:THR:O	4:D:4531:HOH:O	2.14	0.66
1:C:182:GLU:OE1	4:C:3559:HOH:O	2.12	0.66
1:D:55:GLU:HB2	1:D:58:GLU:HG3	1.76	0.66
1:B:112:GLY:HA3	1:B:154:VAL:CG2	2.24	0.65
1:A:317:PHE:CE1	1:A:319:LEU:HD21	2.31	0.65
1:G:118:GLN:HG3	1:G:119:PRO:HD2	1.79	0.65
1:E:209:ASP:HB3	1:G:356:SER:O	1.97	0.65
1:D:403:ALA:HA	1:D:408:THR:HG23	1.79	0.65
1:B:110:ALA:HB2	1:B:219:ILE:HG12	1.77	0.65
1:G:413:ILE:HD11	1:G:435:GLY:CA	2.27	0.65
1:E:28:LEU:HD11	1:E:444:ILE:HD11	1.78	0.64
1:E:71:GLY:CA	1:E:204:ILE:CG2	2.72	0.64
1:F:105:GLY:HA3	4:F:591:HOH:O	1.97	0.64
1:G:29:SER:HB3	1:G:143:ASN:HD21	1.63	0.64
1:E:181:GLU:HG2	1:G:334:LYS:HE2	1.80	0.64
1:F:57:HIS:O	1:F:123:LYS:HE2	1.97	0.63
1:G:403:ALA:HA	1:G:408:THR:HG22	1.80	0.63
1:F:406:VAL:O	1:F:408:THR:HG23	1.99	0.63
1:D:123:LYS:HD3	4:D:4510:HOH:O	1.99	0.62
1:F:36:ASN:HD22	1:F:432:ILE:HD12	1.64	0.62
1:A:339:GLU:OE2	1:A:342:ARG:NH1	2.31	0.62
1:E:88:VAL:O	1:E:88:VAL:HG13	1.99	0.62
1:A:30:ILE:HG12	1:A:436:PHE:HE2	1.65	0.61
1:F:317:PHE:CE1	1:F:319:LEU:HD21	2.35	0.61
1:G:413:ILE:HD11	1:G:435:GLY:HA3	1.82	0.61
1:B:99:VAL:HG21	4:B:1533:HOH:O	2.01	0.61
1:F:118:GLN:HG3	1:F:119:PRO:HD3	1.82	0.60
1:E:63:ARG:HH12	1:E:115:LEU:HB3	1.65	0.60
1:E:118:GLN:HG3	1:E:119:PRO:CD	2.24	0.60
1:E:30:ILE:HG21	1:E:436:PHE:HE2	1.66	0.60
1:C:128:LEU:HD13	1:C:225:LEU:HG	1.83	0.60
1:D:55:GLU:HB2	1:D:58:GLU:CG	2.32	0.60
1:F:59:PHE:O	1:F:123:LYS:HE3	2.01	0.59
1:A:317:PHE:HE1	1:A:319:LEU:HD21	1.67	0.59
1:G:184:TYR:O	1:G:196:SER:HB2	2.02	0.59
1:F:25:ALA:O	4:F:576:HOH:O	2.17	0.59
1:E:317:PHE:CE1	1:E:319:LEU:HD21	2.38	0.59
1:D:413:ILE:HD11	1:D:435:GLY:HA3	1.83	0.59
1:B:128:LEU:HD13	1:B:225:LEU:HG	1.83	0.59
1:E:74:ARG:HB3	1:E:206:TYR:CZ	2.38	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:120:GLU:HG2	1:H:423:TYR:CZ	2.39	0.58
1:H:367:PHE:CE2	1:H:410:MET:HG3	2.38	0.58
1:C:35:LEU:HB2	1:C:135:GLU:HG3	1.86	0.58
1:C:135:GLU:OE1	1:C:138:ARG:NH1	2.32	0.58
1:H:37:GLN:O	1:H:41:GLU:HG3	2.03	0.58
1:A:120:GLU:HG2	1:A:423:TYR:CZ	2.38	0.58
1:E:35:LEU:HD12	1:E:436:PHE:HB2	1.85	0.58
1:D:60:GLY:HA3	1:D:423:TYR:CD2	2.38	0.58
1:E:137:LEU:HD11	1:E:153:VAL:HG23	1.86	0.58
1:G:49:VAL:HG12	1:G:50:ALA:N	2.18	0.58
1:F:242:ILE:HD12	1:F:375:VAL:HG12	1.85	0.58
1:G:368:HIS:O	1:G:372:ILE:HG12	2.04	0.58
1:E:219:ILE:HD11	1:E:406:VAL:HG21	1.85	0.57
1:D:413:ILE:HD11	1:D:435:GLY:HA2	1.84	0.57
1:E:123:LYS:HE2	1:E:124:TYR:CE1	2.39	0.57
1:A:62:ARG:HD3	4:A:2609:HOH:O	2.04	0.57
1:C:277:MET:HE1	1:C:343:LEU:O	2.04	0.57
1:H:134:LEU:HG	1:H:138:ARG:HD2	1.85	0.57
1:G:159:GLU:OE1	4:G:8505:HOH:O	2.17	0.57
1:B:27:PRO:HG2	1:G:328:VAL:HG22	1.84	0.57
1:G:184:TYR:HA	1:G:197:VAL:HG22	1.86	0.56
1:D:158:ASN:HB3	1:D:169:THR:HG23	1.86	0.56
1:A:308:VAL:HG23	4:A:2542:HOH:O	2.05	0.56
1:F:229:GLN:HG2	1:F:420:SER:OG	2.06	0.56
1:E:39:ILE:HG22	1:E:131:LEU:HD12	1.87	0.56
1:D:128:LEU:HD13	1:D:225:LEU:HG	1.89	0.55
1:F:135:GLU:O	1:F:139:THR:CG2	2.54	0.55
1:H:19:THR:O	1:H:19:THR:HG23	2.07	0.55
1:F:238:LYS:HD2	1:F:389:ARG:HB2	1.88	0.55
1:E:296:PHE:HE1	1:E:319:LEU:HD22	1.71	0.55
1:D:59:PHE:O	1:D:123:LYS:HD2	2.07	0.55
1:E:291:ARG:HH11	1:E:291:ARG:HB2	1.72	0.54
1:G:49:VAL:HG12	1:G:50:ALA:H	1.72	0.54
1:H:211:PRO:HG2	1:H:216:GLU:HG2	1.88	0.54
1:E:296:PHE:CE1	1:E:319:LEU:HD22	2.42	0.54
1:C:250:ASN:HD21	1:C:252:GLN:HE21	1.55	0.54
1:H:63:ARG:CZ	1:H:73:MET:HG3	2.38	0.54
1:B:175:SER:O	1:B:176:HIS:HB2	2.07	0.54
1:A:414:PRO:HD2	1:A:431:GLU:HG2	1.90	0.54
1:E:96:MET:SD	1:E:206:TYR:CE2	3.01	0.53
1:E:301:ILE:HD12	1:E:317:PHE:HB3	1.90	0.53
1:A:101:PRO:HA	1:A:150:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:371:CYS:HB3	1:C:409:SER:CB	2.38	0.53
1:A:135:GLU:HG2	4:A:2564:HOH:O	2.07	0.53
1:F:455:HIS:N	1:F:455:HIS:HD2	2.04	0.53
1:B:371:CYS:HB3	1:B:409:SER:CB	2.36	0.53
1:E:93:ILE:HG13	1:E:173:VAL:HG21	1.91	0.53
1:E:123:LYS:HE2	1:E:124:TYR:HE1	1.74	0.53
1:A:204:ILE:HD12	1:A:206:TYR:CD1	2.44	0.53
1:D:222:HIS:HB3	1:D:408:THR:HB	1.91	0.52
1:G:240:ILE:HG12	1:G:438:VAL:HG21	1.91	0.52
1:H:371:CYS:CB	1:H:409:SER:HB2	2.40	0.52
1:G:247:GLN:HE21	1:G:324:PRO:HD3	1.74	0.52
1:E:233:LEU:HD22	1:E:238:LYS:HB2	1.91	0.52
1:F:35:LEU:HB2	1:F:135:GLU:HG3	1.92	0.52
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.74	0.52
1:G:317:PHE:HE1	1:G:319:LEU:HD21	1.74	0.52
1:B:101:PRO:HA	1:B:150:ASP:OD1	2.10	0.52
1:B:247:GLN:HE21	1:B:324:PRO:HD3	1.75	0.52
1:E:34:ARG:HD3	1:E:135:GLU:OE1	2.10	0.52
1:A:30:ILE:HD11	1:A:440:LEU:CD2	2.40	0.52
1:F:371:CYS:HB3	1:F:409:SER:HB2	1.92	0.52
1:E:211:PRO:O	1:E:217:ASN:CG	2.49	0.51
1:E:222:HIS:HB3	1:E:408:THR:HG22	1.92	0.51
1:G:175:SER:OG	1:G:401:GLN:O	2.27	0.51
1:A:403:ALA:HA	1:A:408:THR:HG23	1.93	0.51
1:E:291:ARG:HH11	1:E:291:ARG:CB	2.23	0.51
1:F:292:HIS:HE1	1:F:335:GLU:OE1	1.93	0.51
1:B:296:PHE:HE1	1:B:319:LEU:HB3	1.74	0.51
1:C:37:GLN:O	1:C:41:GLU:CG	2.58	0.51
1:F:54:GLN:HG2	4:F:555:HOH:O	2.10	0.51
1:A:204:ILE:HD12	1:A:206:TYR:HD1	1.75	0.51
1:H:135:GLU:HB3	1:H:436:PHE:CE1	2.46	0.51
1:E:137:LEU:HD11	1:E:153:VAL:CG2	2.41	0.51
1:H:227:ILE:HA	1:H:413:ILE:HD13	1.92	0.51
1:G:74:ARG:HB3	1:G:206:TYR:CZ	2.46	0.51
1:F:317:PHE:HE1	1:F:319:LEU:HD21	1.74	0.50
1:H:51:ARG:NH1	1:H:53:GLY:O	2.41	0.50
1:D:240:ILE:HG12	1:D:438:VAL:HG21	1.92	0.50
1:D:114:HIS:HB2	1:D:116:ASP:OD1	2.11	0.50
1:G:166:ARG:HG3	1:G:166:ARG:HH11	1.76	0.50
1:G:413:ILE:HD11	1:G:435:GLY:HA2	1.92	0.50
1:A:449:TYR:HA	1:A:452:ILE:HD12	1.93	0.50
1:C:93:ILE:HG13	1:C:173:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:20:LEU:O	1:F:377:ARG:NH1	2.43	0.50
1:D:166:ARG:O	1:D:169:THR:HG22	2.10	0.50
1:G:171:SER:O	1:G:175:SER:HB2	2.11	0.50
1:D:238:LYS:HD2	1:D:389:ARG:HB2	1.92	0.50
1:D:175:SER:O	1:D:176:HIS:HB2	2.12	0.50
1:E:30:ILE:HG22	1:E:436:PHE:HE2	1.75	0.50
1:A:204:ILE:HD12	1:A:206:TYR:HB2	1.93	0.50
1:G:446:TYR:CE2	1:G:450:ARG:HD2	2.47	0.50
1:H:346:ILE:HD13	1:H:346:ILE:N	2.27	0.49
1:H:403:ALA:N	1:H:404:PRO:CD	2.75	0.49
1:A:371:CYS:HB3	1:A:409:SER:CB	2.42	0.49
1:C:267:PRO:HB2	4:C:3548:HOH:O	2.11	0.49
1:B:92:LYS:HD2	1:B:211:PRO:HA	1.94	0.49
1:E:88:VAL:O	1:E:88:VAL:CG1	2.61	0.49
1:F:111:THR:O	1:F:153:VAL:HA	2.12	0.49
1:G:238:LYS:HD2	1:G:389:ARG:HB2	1.94	0.49
1:A:236:GLU:OE2	1:B:269:ARG:NH2	2.45	0.49
1:C:172:SER:HA	1:C:401:GLN:HE21	1.78	0.49
1:G:403:ALA:HA	1:G:408:THR:CG2	2.43	0.49
1:H:371:CYS:HB3	1:H:409:SER:HB2	1.95	0.49
1:B:169:THR:O	1:B:173:VAL:HG13	2.11	0.49
1:B:26:ALA:HB2	1:G:291:ARG:O	2.13	0.49
1:E:34:ARG:CZ	1:E:138:ARG:HD2	2.42	0.49
1:C:378:SER:OG	1:C:441:GLN:HB3	2.11	0.49
1:E:233:LEU:HD21	1:E:391:ILE:HD11	1.94	0.48
1:A:222:HIS:O	1:A:408:THR:HB	2.13	0.48
1:E:214:TYR:H	1:E:214:TYR:HD1	1.61	0.48
1:A:371:CYS:CB	1:A:409:SER:HB2	2.43	0.48
1:E:211:PRO:O	1:E:217:ASN:OD1	2.31	0.48
1:C:371:CYS:CB	1:C:409:SER:HB2	2.43	0.48
1:D:269:ARG:HH11	1:D:269:ARG:HG2	1.77	0.48
1:H:406:VAL:HG23	1:H:408:THR:HG22	1.96	0.48
1:G:317:PHE:CE1	1:G:319:LEU:HD21	2.49	0.48
1:H:227:ILE:HG22	1:H:413:ILE:HD11	1.96	0.48
1:A:192:ASP:O	1:A:194:PRO:HD3	2.14	0.48
1:G:111:THR:O	1:G:153:VAL:HA	2.14	0.47
1:F:249:TYR:CE2	1:F:362:SER:HB3	2.49	0.47
1:A:159:GLU:HG2	1:A:168:CYS:SG	2.54	0.47
1:E:115:LEU:HD21	1:E:130:VAL:HG21	1.96	0.47
1:A:34:ARG:HG2	1:A:135:GLU:OE1	2.13	0.47
1:H:57:HIS:O	1:H:123:LYS:HE2	2.15	0.47
1:A:402:THR:OG1	1:A:408:THR:HG21	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:122:GLY:HA3	1:E:425:GLU:HB3	1.96	0.47
1:A:33:GLY:O	1:A:37:GLN:HG2	2.14	0.47
1:H:240:ILE:HG12	1:H:438:VAL:HG21	1.96	0.47
1:B:287:GLU:HG3	4:B:1549:HOH:O	2.15	0.47
1:D:403:ALA:HA	1:D:408:THR:CG2	2.45	0.47
1:B:440:LEU:O	1:B:444:ILE:HG13	2.15	0.47
1:E:317:PHE:HE1	1:E:319:LEU:HD21	1.77	0.46
1:H:402:THR:OG1	1:H:408:THR:HG21	2.16	0.46
1:F:249:TYR:OH	1:F:360:GLN:NE2	2.47	0.46
1:A:250:ASN:HD22	1:A:250:ASN:C	2.18	0.46
1:G:60:GLY:HA3	1:G:423:TYR:CD2	2.50	0.46
1:E:78:THR:CG2	1:E:88:VAL:HG11	2.35	0.46
1:E:30:ILE:HG21	1:E:436:PHE:CE2	2.49	0.46
1:A:18:GLY:HA2	1:A:22:LEU:HD13	1.96	0.46
1:H:111:THR:O	1:H:153:VAL:HA	2.14	0.46
1:A:339:GLU:CD	1:A:342:ARG:NH1	2.69	0.46
1:H:46:PHE:CD1	1:H:73:MET:HG2	2.50	0.46
1:A:277:MET:HG3	1:A:352:LEU:HD22	1.96	0.46
1:E:246:VAL:HG21	1:E:400:CYS:SG	2.55	0.46
1:G:113:SER:HB3	1:G:130:VAL:HG23	1.98	0.46
1:C:403:ALA:HA	1:C:408:THR:HG23	1.96	0.46
1:H:232:ILE:O	1:H:236:GLU:HG3	2.16	0.46
1:F:259:VAL:HG23	1:F:272:LYS:HD2	1.98	0.46
1:B:406:VAL:HG23	1:B:408:THR:HG22	1.97	0.46
1:E:74:ARG:HB3	1:E:206:TYR:OH	2.16	0.45
1:C:406:VAL:HG23	1:C:408:THR:HG22	1.97	0.45
1:B:111:THR:O	1:B:153:VAL:HA	2.17	0.45
1:C:100:TYR:HA	1:C:101:PRO:HD3	1.81	0.45
1:B:234:GLU:OE2	1:B:417:ASP:N	2.46	0.45
1:E:38:THR:HG21	1:E:138:ARG:HH22	1.81	0.45
1:C:74:ARG:HB3	1:C:206:TYR:CZ	2.51	0.45
1:E:111:THR:O	1:E:153:VAL:HA	2.16	0.45
1:B:236:GLU:OE1	1:B:389:ARG:HD2	2.16	0.45
1:F:36:ASN:ND2	1:F:432:ILE:HD12	2.31	0.45
1:H:168:CYS:O	1:H:172:SER:OG	2.32	0.45
1:A:281:MET:HE3	1:A:344:ILE:HD13	1.98	0.45
1:C:171:SER:O	1:C:175:SER:HB2	2.16	0.45
1:B:292:HIS:HE1	1:B:335:GLU:OE1	2.00	0.45
1:B:136:VAL:HG21	1:B:443:ILE:HD11	1.99	0.45
1:H:96:MET:HG3	1:H:155:VAL:HB	1.99	0.45
1:A:35:LEU:HB2	1:A:135:GLU:HG3	1.99	0.45
1:E:297:THR:OG1	1:F:271:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:118:GLN:HE22	1:F:421:HIS:CE1	2.34	0.45
1:G:111:THR:HG23	1:G:439:LEU:HD11	1.98	0.45
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.76	0.45
1:B:55:GLU:HB2	1:B:58:GLU:CG	2.34	0.45
1:F:118:GLN:NE2	1:F:421:HIS:CE1	2.85	0.45
1:F:204:ILE:HD12	1:F:206:TYR:CD1	2.51	0.45
1:C:30:ILE:HD11	1:C:440:LEU:HD22	1.99	0.44
1:G:246:VAL:HG22	1:G:393:SER:HB3	1.98	0.44
1:A:445:ASN:HD22	1:A:445:ASN:HA	1.64	0.44
1:H:30:ILE:HG13	1:H:30:ILE:O	2.17	0.44
1:D:246:VAL:HG21	1:D:400:CYS:SG	2.57	0.44
1:C:154:VAL:HG11	1:C:156:TRP:CE2	2.53	0.44
1:C:176:HIS:HE1	1:C:213:SER:OG	2.00	0.44
1:F:128:LEU:HD21	1:F:432:ILE:HG23	1.99	0.44
1:F:45:GLN:HG2	1:F:46:PHE:CE1	2.52	0.44
1:D:157:PHE:CE1	1:D:201:LEU:HD21	2.52	0.44
1:G:268:TRP:CE2	1:H:290:GLN:HG2	2.53	0.44
1:A:277:MET:CG	1:A:352:LEU:HD22	2.47	0.44
1:H:323:HIS:CG	1:H:324:PRO:HD2	2.52	0.44
1:G:310:ILE:HD12	4:G:8520:HOH:O	2.18	0.44
1:E:245:GLY:HA2	1:E:367:PHE:CD1	2.53	0.44
1:D:163:ARG:NH1	1:D:191:GLU:OE1	2.51	0.44
1:C:30:ILE:HG12	1:C:436:PHE:HE2	1.82	0.43
1:G:176:HIS:HA	4:G:8523:HOH:O	2.17	0.43
1:H:317:PHE:HE1	1:H:319:LEU:HD21	1.80	0.43
1:H:281:MET:CE	1:H:344:ILE:HG23	2.48	0.43
1:G:323:HIS:ND1	1:G:324:PRO:HD2	2.33	0.43
1:H:107:LYS:HG3	1:H:107:LYS:H	1.55	0.43
1:D:111:THR:O	1:D:153:VAL:HA	2.19	0.43
1:C:73:MET:CE	1:C:115:LEU:HD22	2.49	0.43
1:H:120:GLU:HG2	1:H:423:TYR:CE2	2.54	0.43
1:E:99:VAL:HG12	1:E:99:VAL:O	2.18	0.43
1:B:93:ILE:HG23	1:B:93:ILE:O	2.19	0.43
1:F:371:CYS:CB	1:F:409:SER:HB2	2.47	0.43
1:G:189:VAL:HG12	1:G:190:GLY:H	1.83	0.43
1:A:113:SER:HB3	1:A:130:VAL:HG12	2.01	0.43
1:C:113:SER:HB3	1:C:130:VAL:HG23	1.99	0.43
1:A:169:THR:O	1:A:173:VAL:HG23	2.19	0.43
1:G:107:LYS:O	1:G:450:ARG:NH2	2.50	0.43
1:C:406:VAL:O	1:C:408:THR:HG23	2.19	0.43
1:B:222:HIS:O	1:B:408:THR:HB	2.19	0.43
1:E:117:THR:HB	1:E:121:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:ASP:OD2	1:A:401:GLN:NE2	2.52	0.43
1:D:52:TRP:CZ2	1:D:58:GLU:HA	2.54	0.43
1:E:291:ARG:HH11	1:E:291:ARG:CG	2.32	0.43
1:B:108:PRO:HG2	1:B:219:ILE:HG13	2.01	0.43
1:E:156:TRP:HZ3	1:E:222:HIS:NE2	2.16	0.43
1:A:89:LYS:CD	1:A:210:THR:HG21	2.49	0.43
1:G:247:GLN:NE2	1:G:324:PRO:HD3	2.33	0.42
1:B:445:ASN:HD22	1:B:445:ASN:HA	1.69	0.42
1:D:117:THR:HB	1:D:121:ALA:CB	2.48	0.42
1:A:236:GLU:OE2	1:A:389:ARG:NH1	2.52	0.42
1:A:91:ASP:HB2	1:A:210:THR:O	2.20	0.42
1:C:344:ILE:HG23	1:C:345:LYS:HD3	1.99	0.42
1:E:124:TYR:CD2	1:E:432:ILE:HD11	2.55	0.42
1:H:371:CYS:HB2	1:H:409:SER:HB2	2.02	0.42
1:B:168:CYS:O	1:B:172:SER:HB2	2.20	0.42
1:E:271:ARG:CZ	1:E:311:ILE:HD11	2.50	0.42
1:D:252:GLN:HB2	4:D:4554:HOH:O	2.20	0.42
1:A:296:PHE:CE1	1:A:319:LEU:HD22	2.54	0.42
1:B:262:HIS:HB3	1:B:265:THR:OG1	2.19	0.42
1:C:63:ARG:HB3	1:C:117:THR:HG23	2.01	0.42
1:A:30:ILE:HD11	1:A:440:LEU:HD22	2.01	0.42
1:F:171:SER:OG	1:F:398:ASP:OD1	2.37	0.42
1:C:318:THR:C	1:C:319:LEU:HD23	2.40	0.42
1:F:288:ILE:HG13	1:F:291:ARG:NH2	2.34	0.42
1:C:362:SER:HA	1:C:363:PRO:HD3	1.79	0.42
1:C:414:PRO:HG2	1:C:431:GLU:CD	2.39	0.42
1:H:378:SER:OG	1:H:441:GLN:HB3	2.19	0.42
1:F:172:SER:HA	1:F:401:GLN:HG3	2.02	0.42
1:E:93:ILE:O	1:E:93:ILE:HG23	2.20	0.42
1:C:111:THR:O	1:C:153:VAL:HA	2.19	0.42
1:G:175:SER:HB3	1:G:177:ASP:OD2	2.19	0.42
1:G:49:VAL:CG1	1:G:50:ALA:N	2.83	0.41
1:G:296:PHE:HE1	1:G:319:LEU:HD22	1.85	0.41
1:D:189:VAL:CG2	1:D:190:GLY:N	2.73	0.41
1:G:298:CYS:SG	1:G:317:PHE:HB2	2.60	0.41
1:C:402:THR:OG1	1:C:408:THR:HG21	2.20	0.41
1:B:403:ALA:HA	1:B:408:THR:HG23	2.02	0.41
1:F:268:TRP:HA	1:F:271:ARG:HD3	2.02	0.41
1:G:290:GLN:HG3	1:H:268:TRP:CE2	2.55	0.41
1:E:127:ILE:H	1:E:127:ILE:HG12	1.53	0.41
1:C:290:GLN:HG2	1:D:268:TRP:CE2	2.55	0.41
1:H:74:ARG:HB3	1:H:206:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:402:THR:OG1	1:D:408:THR:HG21	2.20	0.41
1:H:127:ILE:H	1:H:127:ILE:HG12	1.62	0.41
1:G:398:ASP:N	1:G:398:ASP:OD1	2.44	0.41
1:G:339:GLU:OE2	1:G:342:ARG:NH1	2.52	0.41
1:C:78:THR:HB	1:C:88:VAL:HG11	2.01	0.41
1:B:319:LEU:N	1:B:319:LEU:HD23	2.36	0.41
1:A:22:LEU:HD11	1:A:449:TYR:HB2	2.02	0.41
1:B:242:ILE:HD12	1:B:375:VAL:HG12	2.02	0.41
1:A:111:THR:O	1:A:153:VAL:HA	2.21	0.41
1:B:443:ILE:H	1:B:443:ILE:HG12	1.71	0.41
1:H:192:ASP:O	1:H:194:PRO:HD3	2.21	0.41
1:G:181:GLU:H	1:G:181:GLU:HG3	1.57	0.41
1:E:38:THR:HG21	1:E:138:ARG:NH2	2.36	0.41
1:E:260:GLY:HA2	1:E:311:ILE:O	2.21	0.41
1:F:30:ILE:HD11	1:F:440:LEU:CD2	2.50	0.41
1:G:223:PHE:CE2	1:G:442:ALA:HB1	2.56	0.41
1:E:224:GLU:HB3	1:E:410:MET:HG2	2.03	0.41
1:G:54:GLN:HE21	1:G:54:GLN:HB3	1.70	0.41
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.90	0.41
1:D:240:ILE:HD13	1:D:383:PHE:CE1	2.56	0.41
1:G:413:ILE:CD1	1:G:435:GLY:HA3	2.50	0.40
1:H:87:LYS:HB2	1:H:87:LYS:NZ	2.36	0.40
1:D:166:ARG:NH1	1:D:167:SER:O	2.55	0.40
1:D:260:GLY:HA2	1:D:311:ILE:O	2.22	0.40
1:H:38:THR:O	1:H:42:THR:HG23	2.21	0.40
1:E:38:THR:HA	1:E:41:GLU:HG2	2.02	0.40
1:H:77:PHE:CD2	1:H:96:MET:CE	3.04	0.40
1:E:125:ASP:O	1:E:127:ILE:HG12	2.22	0.40
1:B:361:VAL:N	4:B:1525:HOH:O	2.49	0.40
1:B:46:PHE:O	1:B:63:ARG:HD3	2.21	0.40
1:A:238:LYS:HD3	1:A:386:ASP:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

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	436/462 (94%)	420 (96%)	16 (4%)	0	100	100
1	B	431/462 (93%)	418 (97%)	11 (3%)	2 (0%)	38	70
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	38	70
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	25	55
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	38	70
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	38	70
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	25	55
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	56	86
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	38	70

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	B	106	GLY
1	B	454	GLY
1	C	21	ASN
1	C	106	GLY
1	D	25	ALA
1	E	106	GLY
1	F	106	GLY
1	G	106	GLY
1	G	189	VAL
1	G	190	GLY
1	H	106	GLY
1	D	106	GLY
1	F	192	ASP
1	G	191	GLU
1	E	454	GLY
1	D	189	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	360/383 (94%)	323 (90%)	37 (10%)	10	23
1	B	356/383 (93%)	314 (88%)	42 (12%)	8	18
1	C	360/383 (94%)	332 (92%)	28 (8%)	18	40
1	D	360/383 (94%)	317 (88%)	43 (12%)	8	18
1	E	356/383 (93%)	284 (80%)	72 (20%)	2	5
1	F	360/383 (94%)	321 (89%)	39 (11%)	9	21
1	G	355/383 (93%)	289 (81%)	66 (19%)	2	6
1	H	360/383 (94%)	325 (90%)	35 (10%)	12	27
All	All	2867/3064 (94%)	2505 (87%)	362 (13%)	7	16

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	30	ILE
1	A	32	SER
1	A	51	ARG
1	A	62	ARG
1	A	78	THR
1	A	79	ASN
1	A	87	LYS
1	A	93	ILE
1	A	134	LEU
1	A	163	ARG
1	A	166	ARG
1	A	175	SER
1	A	192	ASP
1	A	193	LYS
1	A	200	SER
1	A	202	LYS
1	A	204	ILE
1	A	210	THR
1	A	240	ILE
1	A	247	GLN

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	253	LYS
1	A	271	ARG
1	A	291	ARG
1	A	325	SER
1	A	334	LYS
1	A	348	ASP
1	A	361	VAL
1	A	373	GLU
1	A	377	ARG
1	A	384	LYS
1	A	385	LYS
1	A	408	THR
1	A	416	LYS
1	A	433	GLU
1	A	445	ASN
1	B	29	SER
1	B	30	ILE
1	B	37	GLN
1	B	82	GLU
1	B	87	LYS
1	B	89	LYS
1	B	93	ILE
1	B	113	SER
1	B	128	LEU
1	B	134	LEU
1	B	135	GLU
1	B	139	THR
1	B	163	ARG
1	B	193	LYS
1	B	201	LEU
1	B	202	LYS
1	B	219	ILE
1	B	237	ASN
1	B	244	THR
1	B	250	ASN
1	B	271	ARG
1	B	286	SER
1	B	287	GLU
1	B	307	SER
1	B	309	ASN
1	B	319	LEU

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Mol	Chain	Res	Type
1	B	345	LYS
1	B	356	SER
1	B	362	SER
1	B	369	GLU
1	B	376	SER
1	B	377	ARG
1	B	389	ARG
1	B	390	GLN
1	B	408	THR
1	B	415	SER
1	B	419	LEU
1	B	420	SER
1	B	428	SER
1	B	433	GLU
1	B	443	ILE
1	B	455	HIS
1	C	30	ILE
1	C	32	SER
1	C	73	MET
1	C	78	THR
1	C	87	LYS
1	C	93	ILE
1	C	103	LYS
1	C	107	LYS
1	C	128	LEU
1	C	134	LEU
1	C	141	LYS
1	C	171	SER
1	C	176	HIS
1	C	209	ASP
1	C	240	ILE
1	C	250	ASN
1	C	252	GLN
1	C	286	SER
1	C	316	SER
1	C	325	SER
1	C	356	SER
1	C	362	SER
1	C	408	THR
1	C	415	SER
1	C	419	LEU
1	C	428	SER

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Mol	Chain	Res	Type
1	C	443	ILE
1	C	453	ARG
1	D	32	SER
1	D	37	GLN
1	D	45	GLN
1	D	49	VAL
1	D	54	GLN
1	D	62	ARG
1	D	78	THR
1	D	87	LYS
1	D	89	LYS
1	D	93	ILE
1	D	107	LYS
1	D	123	LYS
1	D	128	LEU
1	D	141	LYS
1	D	142	ASP
1	D	146	VAL
1	D	169	THR
1	D	191	GLU
1	D	192	ASP
1	D	193	LYS
1	D	202	LYS
1	D	216	GLU
1	D	234	GLU
1	D	236	GLU
1	D	240	ILE
1	D	244	THR
1	D	252	GLN
1	D	319	LEU
1	D	325	SER
1	D	332	MET
1	D	345	LYS
1	D	362	SER
1	D	373	GLU
1	D	384	LYS
1	D	385	LYS
1	D	386	ASP
1	D	390	GLN
1	D	408	THR
1	D	430	GLU
1	D	440	LEU

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Mol	Chain	Res	Type
1	D	447	ASP
1	D	452	ILE
1	D	453	ARG
1	E	29	SER
1	E	30	ILE
1	E	35	LEU
1	E	39	ILE
1	E	40	LEU
1	E	45	GLN
1	E	49	VAL
1	E	55	GLU
1	E	56	SER
1	E	73	MET
1	E	81	CYS
1	E	87	LYS
1	E	90	VAL
1	E	92	LYS
1	E	93	ILE
1	E	96	MET
1	E	99	VAL
1	E	103	LYS
1	E	107	LYS
1	E	113	SER
1	E	115	LEU
1	E	127	ILE
1	E	139	THR
1	E	150	ASP
1	E	152	CYS
1	E	154	VAL
1	E	156	TRP
1	E	159	GLU
1	E	160	GLU
1	E	167	SER
1	E	171	SER
1	E	176	HIS
1	E	177	ASP
1	E	180	LEU
1	E	184	TYR
1	E	186	LEU
1	E	188	SER
1	E	189	VAL
1	E	192	ASP

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Mol	Chain	Res	Type
1	E	193	LYS
1	E	195	GLU
1	E	200	SER
1	E	202	LYS
1	E	207	ILE
1	E	214	TYR
1	E	215	LYS
1	E	216	GLU
1	E	217	ASN
1	E	237	ASN
1	E	240	ILE
1	E	250	ASN
1	E	252	GLN
1	E	253	LYS
1	E	286	SER
1	E	287	GLU
1	E	291	ARG
1	E	301	ILE
1	E	325	SER
1	E	334	LYS
1	E	345	LYS
1	E	356	SER
1	E	377	ARG
1	E	385	LYS
1	E	391	ILE
1	E	406	VAL
1	E	413	ILE
1	E	416	LYS
1	E	417	ASP
1	E	433	GLU
1	E	440	LEU
1	E	441	GLN
1	E	444	ILE
1	F	19	THR
1	F	30	ILE
1	F	32	SER
1	F	49	VAL
1	F	51	ARG
1	F	54	GLN
1	F	83	SER
1	F	89	LYS
1	F	93	ILE

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Mol	Chain	Res	Type
1	F	103	LYS
1	F	118	GLN
1	F	128	LEU
1	F	134	LEU
1	F	139	THR
1	F	141	LYS
1	F	163	ARG
1	F	192	ASP
1	F	193	LYS
1	F	202	LYS
1	F	203	ASN
1	F	240	ILE
1	F	250	ASN
1	F	271	ARG
1	F	286	SER
1	F	288	ILE
1	F	345	LYS
1	F	346	ILE
1	F	348	ASP
1	F	356	SER
1	F	358	THR
1	F	361	VAL
1	F	377	ARG
1	F	384	LYS
1	F	385	LYS
1	F	387	GLN
1	F	401	GLN
1	F	420	SER
1	F	437	LYS
1	F	455	HIS
1	G	28	LEU
1	G	34	ARG
1	G	37	GLN
1	G	54	GLN
1	G	62	ARG
1	G	63	ARG
1	G	82	GLU
1	G	83	SER
1	G	87	LYS
1	G	92	LYS
1	G	93	ILE
1	G	103	LYS

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Mol	Chain	Res	Type
1	G	107	LYS
1	G	128	LEU
1	G	135	GLU
1	G	141	LYS
1	G	142	ASP
1	G	144	ASN
1	G	146	VAL
1	G	167	SER
1	G	175	SER
1	G	177	ASP
1	G	181	GLU
1	G	193	LYS
1	G	197	VAL
1	G	200	SER
1	G	203	ASN
1	G	207	ILE
1	G	210	THR
1	G	215	LYS
1	G	216	GLU
1	G	227	ILE
1	G	228	GLU
1	G	234	GLU
1	G	240	ILE
1	G	250	ASN
1	G	252	GLN
1	G	269	ARG
1	G	287	GLU
1	G	293	ASN
1	G	316	SER
1	G	322	ARG
1	G	325	SER
1	G	332	MET
1	G	342	ARG
1	G	345	LYS
1	G	356	SER
1	G	359	LEU
1	G	361	VAL
1	G	369	GLU
1	G	376	SER
1	G	377	ARG
1	G	384	LYS
1	G	386	ASP

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Mol	Chain	Res	Type
1	G	389	ARG
1	G	390	GLN
1	G	391	ILE
1	G	398	ASP
1	G	415	SER
1	G	416	LYS
1	G	419	LEU
1	G	420	SER
1	G	427	SER
1	G	430	GLU
1	G	440	LEU
1	G	444	ILE
1	H	29	SER
1	H	32	SER
1	H	54	GLN
1	H	73	MET
1	H	93	ILE
1	H	96	MET
1	H	103	LYS
1	H	107	LYS
1	H	116	ASP
1	H	123	LYS
1	H	138	ARG
1	H	141	LYS
1	H	175	SER
1	H	189	VAL
1	H	192	ASP
1	H	193	LYS
1	H	215	LYS
1	H	216	GLU
1	H	240	ILE
1	H	250	ASN
1	H	269	ARG
1	H	286	SER
1	H	334	LYS
1	H	344	ILE
1	H	355	GLU
1	H	356	SER
1	H	361	VAL
1	H	384	LYS
1	H	385	LYS
1	H	389	ARG

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Mol	Chain	Res	Type
1	H	399	SER
1	H	408	THR
1	H	413	ILE
1	H	433	GLU
1	H	451	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	158	ASN
1	A	250	ASN
1	A	309	ASN
1	A	390	GLN
1	A	445	ASN
1	A	455	HIS
1	B	176	HIS
1	B	217	ASN
1	B	250	ASN
1	B	290	GLN
1	B	292	HIS
1	B	309	ASN
1	B	382	GLN
1	B	422	ASN
1	B	434	ASN
1	B	445	ASN
1	B	448	ASN
1	C	118	GLN
1	C	176	HIS
1	C	217	ASN
1	C	252	GLN
1	C	360	GLN
1	C	401	GLN
1	C	434	ASN
1	D	176	HIS
1	D	247	GLN
1	D	250	ASN
1	D	252	GLN
1	D	360	GLN
1	D	441	GLN
1	D	445	ASN
1	E	118	GLN

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Mol	Chain	Res	Type
1	E	247	GLN
1	E	250	ASN
1	E	397	HIS
1	E	434	ASN
1	E	441	GLN
1	E	445	ASN
1	F	36	ASN
1	F	54	GLN
1	F	118	GLN
1	F	250	ASN
1	F	290	GLN
1	F	292	HIS
1	F	360	GLN
1	F	434	ASN
1	F	455	HIS
1	G	54	GLN
1	G	118	GLN
1	G	143	ASN
1	G	247	GLN
1	G	250	ASN
1	G	401	GLN
1	G	405	HIS
1	G	434	ASN
1	H	247	GLN
1	H	292	HIS
1	H	401	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	BIB	A	2502	-	4,6,6	1.06	0	4,7,7	2.24	1 (25%)
3	BIB	B	1502	-	4,6,6	0.58	0	4,7,7	2.41	2 (50%)
3	BIB	C	3502	-	4,6,6	0.50	0	4,7,7	5.72	1 (25%)
3	BIB	D	4502	-	4,6,6	0.48	0	4,7,7	14.00	2 (50%)
3	BIB	E	5502	-	4,6,6	0.51	0	4,7,7	15.06	1 (25%)
3	BIB	E	6502	-	4,6,6	1.13	1 (25%)	4,7,7	5.00	1 (25%)
3	BIB	G	7502	-	4,6,6	0.42	0	4,7,7	0.52	0
3	BIB	G	8502	-	4,6,6	0.85	0	4,7,7	11.30	1 (25%)

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	BIB	A	2502	-	-	0/2/6/6	0/0/0/0
3	BIB	B	1502	-	-	0/2/6/6	0/0/0/0
3	BIB	C	3502	-	-	0/2/6/6	0/0/0/0
3	BIB	D	4502	-	-	0/2/6/6	0/0/0/0
3	BIB	E	5502	-	-	0/2/6/6	0/0/0/0
3	BIB	E	6502	-	-	0/2/6/6	0/0/0/0
3	BIB	G	7502	-	-	0/2/6/6	0/0/0/0
3	BIB	G	8502	-	-	0/2/6/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6502	BIB	C4-C3	2.08	1.55	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5502	BIB	C4-C3-C5	-30.07	108.46	111.91
3	D	4502	BIB	C4-C3-C5	-27.92	108.71	111.91
3	G	8502	BIB	C4-C3-C5	22.60	114.50	111.91
3	C	3502	BIB	C4-C3-C5	-11.37	110.61	111.91
3	E	6502	BIB	C4-C3-C5	9.96	113.05	111.91
3	A	2502	BIB	C4-C3-C5	4.44	112.42	111.91
3	B	1502	BIB	C4-C3-C5	-4.29	111.42	111.91
3	B	1502	BIB	C3-C4-N1	-2.08	107.22	113.40
3	D	4502	BIB	C3-C4-N1	-2.01	107.44	113.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	438/462 (94%)	0.86	54 (12%) 5 5	12, 16, 19, 29	0
1	B	433/462 (93%)	1.02	66 (15%) 3 3	13, 16, 18, 20	0
1	C	438/462 (94%)	0.71	38 (8%) 10 10	13, 16, 19, 30	0
1	D	437/462 (94%)	1.12	77 (17%) 2 2	14, 16, 17, 20	0
1	E	433/462 (93%)	2.20	198 (45%) 1 0	15, 16, 17, 20	0
1	F	438/462 (94%)	0.67	41 (9%) 9 8	13, 16, 19, 31	0
1	G	430/462 (93%)	2.08	195 (45%) 1 0	13, 16, 17, 20	0
1	H	438/462 (94%)	0.81	47 (10%) 6 6	12, 16, 19, 24	0
All	All	3485/3696 (94%)	1.18	716 (20%) 1 2	12, 16, 18, 31	0

All (716) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	211	PRO	9.2
1	E	176	HIS	8.6
1	B	455	HIS	8.3
1	E	455	HIS	8.0
1	G	53	GLY	7.7
1	G	55	GLU	7.7
1	E	106	GLY	7.4
1	E	68	ALA	7.3
1	G	447	ASP	7.2
1	E	93	ILE	7.2
1	G	454	GLY	7.1
1	E	194	PRO	7.0
1	G	455	HIS	7.0
1	E	177	ASP	6.9
1	E	25	ALA	6.7
1	E	178	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	455	HIS	6.6
1	G	386	ASP	6.6
1	E	199	ASP	6.5
1	D	19	THR	6.5
1	E	201	LEU	6.3
1	E	212	ALA	6.2
1	E	183	ALA	6.1
1	G	30	ILE	6.1
1	E	103	LYS	6.1
1	E	76	TRP	6.1
1	D	192	ASP	6.1
1	E	221	ALA	6.1
1	G	370	VAL	6.1
1	E	192	ASP	6.0
1	G	50	ALA	5.9
1	E	30	ILE	5.9
1	F	455	HIS	5.8
1	G	383	PHE	5.7
1	G	104	ASN	5.7
1	G	394	GLY	5.5
1	G	365	VAL	5.5
1	E	210	THR	5.5
1	D	54	GLN	5.4
1	E	101	PRO	5.4
1	G	388	VAL	5.4
1	E	163	ARG	5.4
1	E	451	VAL	5.3
1	E	69	LEU	5.3
1	B	25	ALA	5.3
1	G	363	PRO	5.3
1	G	223	PHE	5.3
1	E	180	LEU	5.3
1	E	449	TYR	5.3
1	E	24	ALA	5.3
1	G	368	HIS	5.3
1	E	79	ASN	5.3
1	G	33	GLY	5.3
1	G	373	GLU	5.2
1	E	92	LYS	5.2
1	B	192	ASP	5.2
1	E	149	TYR	5.2
1	E	102	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	192	ASP	5.1
1	E	100	TYR	5.1
1	G	444	ILE	5.1
1	G	452	ILE	5.1
1	E	197	VAL	5.1
1	E	204	ILE	5.0
1	E	152	CYS	5.0
1	E	96	MET	5.0
1	D	381	ALA	5.0
1	G	27	PRO	4.9
1	G	100	TYR	4.9
1	D	23	PRO	4.9
1	G	102	GLY	4.9
1	G	377	ARG	4.9
1	E	404	PRO	4.9
1	G	412	PHE	4.9
1	G	32	SER	4.9
1	G	451	VAL	4.9
1	G	426	TYR	4.9
1	G	384	LYS	4.8
1	E	366	ASN	4.8
1	E	33	GLY	4.8
1	F	19	THR	4.8
1	D	193	LYS	4.8
1	G	453	ARG	4.8
1	G	149	TYR	4.8
1	G	364	ALA	4.7
1	E	53	GLY	4.7
1	D	178	LEU	4.7
1	G	395	ALA	4.7
1	B	194	PRO	4.7
1	E	365	VAL	4.7
1	E	368	HIS	4.7
1	G	369	GLU	4.7
1	E	198	TYR	4.7
1	E	118	GLN	4.6
1	D	104	ASN	4.6
1	E	91	ASP	4.6
1	E	54	GLN	4.6
1	D	55	GLU	4.6
1	E	219	ILE	4.6
1	E	86	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	323	HIS	4.6
1	B	54	GLN	4.6
1	E	454	GLY	4.6
1	D	21	ASN	4.5
1	E	386	ASP	4.5
1	E	207	ILE	4.5
1	G	43	GLY	4.5
1	D	451	VAL	4.5
1	E	191	GLU	4.5
1	A	298	CYS	4.5
1	G	414	PRO	4.5
1	G	327	ASP	4.5
1	G	54	GLN	4.5
1	G	230	GLY	4.4
1	E	104	ASN	4.4
1	G	367	PHE	4.4
1	E	193	LYS	4.4
1	E	424	TYR	4.4
1	E	105	GLY	4.4
1	G	366	ASN	4.4
1	H	87	LYS	4.3
1	E	41	GLU	4.3
1	G	31	ALA	4.3
1	E	142	ASP	4.3
1	G	443	ILE	4.3
1	E	151	VAL	4.3
1	E	70	ASP	4.2
1	F	129	GLY	4.2
1	G	112	GLY	4.2
1	D	31	ALA	4.2
1	E	185	GLY	4.2
1	E	55	GLU	4.2
1	A	129	GLY	4.2
1	E	39	ILE	4.2
1	E	174	TRP	4.2
1	E	150	ASP	4.2
1	E	138	ARG	4.2
1	G	381	ALA	4.2
1	C	18	GLY	4.2
1	E	377	ARG	4.2
1	E	110	ALA	4.2
1	G	26	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	4.2
1	E	43	GLY	4.2
1	H	19	THR	4.1
1	G	424	TYR	4.1
1	G	436	PHE	4.1
1	E	385	LYS	4.1
1	B	47	GLY	4.1
1	E	400	CYS	4.1
1	E	52	TRP	4.1
1	G	380	PHE	4.1
1	E	48	GLY	4.1
1	H	454	GLY	4.1
1	E	126	GLY	4.1
1	H	455	HIS	4.1
1	B	454	GLY	4.1
1	C	298	CYS	4.1
1	B	106	GLY	4.0
1	D	454	GLY	4.0
1	A	455	HIS	4.0
1	B	149	TYR	4.0
1	G	396	GLY	4.0
1	E	90	VAL	4.0
1	E	370	VAL	4.0
1	D	190	GLY	4.0
1	G	146	VAL	4.0
1	G	433	GLU	4.0
1	E	381	ALA	4.0
1	E	99	VAL	4.0
1	E	187	MET	4.0
1	A	152	CYS	4.0
1	E	190	GLY	3.9
1	E	184	TYR	3.9
1	B	104	ASN	3.9
1	C	192	ASP	3.9
1	G	385	LYS	3.9
1	E	56	SER	3.9
1	G	408	THR	3.9
1	D	50	ALA	3.9
1	B	101	PRO	3.9
1	G	231	PRO	3.9
1	E	189	VAL	3.9
1	E	182	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	235	ASP	3.8
1	E	369	GLU	3.8
1	D	56	SER	3.8
1	E	97	PHE	3.8
1	A	193	LYS	3.8
1	C	133	GLY	3.8
1	E	220	ASP	3.8
1	D	22	LEU	3.8
1	E	98	ALA	3.8
1	A	126	GLY	3.8
1	G	56	SER	3.8
1	E	164	PHE	3.8
1	B	105	GLY	3.8
1	E	405	HIS	3.8
1	E	200	SER	3.8
1	G	103	LYS	3.8
1	B	30	ILE	3.7
1	H	348	ASP	3.7
1	E	67	THR	3.7
1	E	206	TYR	3.7
1	G	111	THR	3.7
1	E	87	LYS	3.7
1	E	120	GLU	3.7
1	D	20	LEU	3.7
1	E	46	PHE	3.7
1	B	68	ALA	3.6
1	G	57	HIS	3.6
1	A	128	LEU	3.6
1	D	146	VAL	3.6
1	B	100	TYR	3.6
1	G	59	PHE	3.6
1	G	432	ILE	3.6
1	G	51	ARG	3.6
1	G	193	LYS	3.6
1	E	181	GLU	3.6
1	G	392	TRP	3.6
1	F	130	VAL	3.6
1	E	214	TYR	3.6
1	G	177	ASP	3.6
1	G	449	TYR	3.6
1	E	115	LEU	3.6
1	A	111	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	113	SER	3.6
1	H	192	ASP	3.6
1	G	41	GLU	3.6
1	G	334	LYS	3.6
1	D	142	ASP	3.6
1	G	228	GLU	3.6
1	A	132	ALA	3.5
1	E	162	ALA	3.5
1	E	175	SER	3.5
1	G	29	SER	3.5
1	E	208	GLY	3.5
1	E	402	THR	3.5
1	G	379	ALA	3.5
1	C	130	VAL	3.5
1	G	246	VAL	3.5
1	B	452	ILE	3.5
1	G	417	ASP	3.5
1	B	369	GLU	3.5
1	E	367	PHE	3.5
1	G	393	SER	3.5
1	G	239	ALA	3.5
1	C	455	HIS	3.5
1	G	138	ARG	3.5
1	A	439	LEU	3.5
1	B	177	ASP	3.4
1	C	128	LEU	3.4
1	G	144	ASN	3.4
1	G	402	THR	3.4
1	G	81	CYS	3.4
1	F	225	LEU	3.4
1	B	386	ASP	3.4
1	G	101	PRO	3.4
1	G	382	GLN	3.4
1	A	130	VAL	3.4
1	C	19	THR	3.4
1	A	131	LEU	3.4
1	E	384	LYS	3.4
1	E	179	SER	3.4
1	C	132	ALA	3.4
1	G	151	VAL	3.4
1	G	249	TYR	3.4
1	E	84	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	79	ASN	3.3
1	E	23	PRO	3.3
1	E	186	LEU	3.3
1	F	152	CYS	3.3
1	E	215	LYS	3.3
1	F	189	VAL	3.3
1	G	106	GLY	3.3
1	A	127	ILE	3.3
1	C	299	GLY	3.3
1	D	53	GLY	3.3
1	D	199	ASP	3.3
1	D	24	ALA	3.3
1	H	129	GLY	3.3
1	D	32	SER	3.3
1	E	139	THR	3.3
1	H	120	GLU	3.3
1	G	69	LEU	3.3
1	E	75	ASP	3.3
1	E	95	ASN	3.2
1	H	132	ALA	3.2
1	G	143	ASN	3.2
1	G	139	THR	3.2
1	G	105	GLY	3.2
1	G	122	GLY	3.2
1	D	120	GLU	3.2
1	E	72	ALA	3.2
1	D	87	LYS	3.2
1	D	30	ILE	3.2
1	A	133	GLY	3.2
1	C	155	VAL	3.2
1	F	154	VAL	3.2
1	H	130	VAL	3.2
1	G	441	GLN	3.2
1	B	86	CYS	3.2
1	B	56	SER	3.2
1	D	191	GLU	3.2
1	G	448	ASN	3.2
1	C	126	GLY	3.2
1	E	170	GLY	3.2
1	E	89	LYS	3.2
1	C	278	SER	3.2
1	F	128	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	453	ARG	3.2
1	F	18	GLY	3.2
1	E	88	VAL	3.1
1	C	327	ASP	3.1
1	H	111	THR	3.1
1	G	152	CYS	3.1
1	B	377	ARG	3.1
1	F	192	ASP	3.1
1	G	145	TYR	3.1
1	E	45	GLN	3.1
1	E	77	PHE	3.1
1	E	433	GLU	3.1
1	A	225	LEU	3.1
1	F	298	CYS	3.1
1	D	135	GLU	3.1
1	E	109	THR	3.1
1	E	447	ASP	3.1
1	E	450	ARG	3.1
1	G	34	ARG	3.1
1	H	153	VAL	3.1
1	F	190	GLY	3.1
1	G	178	LEU	3.1
1	E	129	GLY	3.1
1	E	73	MET	3.1
1	G	389	ARG	3.1
1	G	52	TRP	3.1
1	E	169	THR	3.1
1	D	34	ARG	3.1
1	A	192	ASP	3.1
1	C	127	ILE	3.1
1	A	299	GLY	3.0
1	B	46	PHE	3.0
1	G	430	GLU	3.0
1	A	20	LEU	3.0
1	G	245	GLY	3.0
1	G	411	ILE	3.0
1	B	32	SER	3.0
1	D	33	GLY	3.0
1	D	66	GLY	3.0
1	G	129	GLY	3.0
1	E	121	ALA	3.0
1	A	223	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	275	LEU	3.0
1	E	165	ALA	3.0
1	G	58	GLU	3.0
1	G	374	CYS	3.0
1	E	216	GLU	3.0
1	H	82	GLU	3.0
1	A	443	ILE	3.0
1	H	126	GLY	3.0
1	A	317	PHE	3.0
1	F	127	ILE	3.0
1	G	362	SER	3.0
1	A	154	VAL	3.0
1	G	78	THR	3.0
1	G	331	THR	3.0
1	F	317	PHE	2.9
1	C	115	LEU	2.9
1	G	148	ASN	2.9
1	G	390	GLN	2.9
1	D	81	CYS	2.9
1	E	423	TYR	2.9
1	B	278	SER	2.9
1	D	49	VAL	2.9
1	H	298	CYS	2.9
1	E	223	PHE	2.9
1	A	318	THR	2.9
1	B	451	VAL	2.9
1	D	384	LYS	2.9
1	B	53	GLY	2.9
1	G	227	ILE	2.9
1	A	275	LEU	2.9
1	E	134	LEU	2.9
1	E	380	PHE	2.9
1	D	52	TRP	2.9
1	E	148	ASN	2.9
1	E	224	GLU	2.9
1	G	214	TYR	2.9
1	D	46	PHE	2.9
1	E	327	ASP	2.9
1	E	146	VAL	2.9
1	G	49	VAL	2.9
1	H	18	GLY	2.9
1	A	279	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	198	TYR	2.9
1	A	411	ILE	2.9
1	C	154	VAL	2.9
1	G	126	GLY	2.9
1	G	437	LYS	2.9
1	A	278	SER	2.9
1	C	317	PHE	2.8
1	A	155	VAL	2.8
1	G	99	VAL	2.8
1	A	110	ALA	2.8
1	F	132	ALA	2.8
1	A	282	ILE	2.8
1	D	105	GLY	2.8
1	D	369	GLU	2.8
1	E	401	GLN	2.8
1	G	440	LEU	2.8
1	F	111	THR	2.8
1	G	375	VAL	2.8
1	G	355	GLU	2.8
1	C	153	VAL	2.8
1	E	246	VAL	2.8
1	D	41	GLU	2.8
1	D	189	VAL	2.8
1	E	374	CYS	2.8
1	D	103	LYS	2.8
1	C	131	LEU	2.8
1	B	31	ALA	2.8
1	F	165	ALA	2.8
1	F	126	GLY	2.7
1	B	179	SER	2.7
1	E	44	SER	2.7
1	G	198	TYR	2.7
1	G	190	GLY	2.7
1	H	443	ILE	2.7
1	G	181	GLU	2.7
1	G	76	TRP	2.7
1	D	101	PRO	2.7
1	E	29	SER	2.7
1	D	221	ALA	2.7
1	G	446	TYR	2.7
1	B	55	GLU	2.7
1	D	64	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	364	ALA	2.7
1	F	133	GLY	2.7
1	G	335	GLU	2.7
1	F	115	LEU	2.7
1	G	391	ILE	2.7
1	D	177	ASP	2.7
1	G	150	ASP	2.7
1	E	375	VAL	2.7
1	G	218	GLU	2.7
1	G	419	LEU	2.7
1	A	153	VAL	2.7
1	C	152	CYS	2.7
1	G	400	CYS	2.7
1	E	108	PRO	2.7
1	F	113	SER	2.7
1	D	102	GLY	2.7
1	C	112	GLY	2.6
1	H	127	ILE	2.6
1	E	34	ARG	2.6
1	G	431	GLU	2.6
1	C	223	PHE	2.6
1	G	79	ASN	2.6
1	G	176	HIS	2.6
1	G	236	GLU	2.6
1	A	113	SER	2.6
1	D	187	MET	2.6
1	G	360	GLN	2.6
1	C	113	SER	2.6
1	E	235	ASP	2.6
1	H	264	GLY	2.6
1	A	442	ALA	2.6
1	B	103	LYS	2.6
1	B	327	ASP	2.6
1	E	156	TRP	2.6
1	B	281	MET	2.6
1	F	443	ILE	2.6
1	G	153	VAL	2.6
1	G	191	GLU	2.6
1	G	387	GLN	2.6
1	E	397	HIS	2.6
1	F	110	ALA	2.6
1	G	438	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	215	LYS	2.5
1	B	50	ALA	2.5
1	F	131	LEU	2.5
1	F	439	LEU	2.5
1	G	85	GLY	2.5
1	D	203	ASN	2.5
1	E	452	ILE	2.5
1	F	318	THR	2.5
1	E	27	PRO	2.5
1	E	81	CYS	2.5
1	G	86	CYS	2.5
1	B	453	ARG	2.5
1	D	47	GLY	2.5
1	B	276	LEU	2.5
1	C	439	LEU	2.5
1	E	32	SER	2.5
1	E	196	SER	2.5
1	B	24	ALA	2.5
1	D	327	ASP	2.5
1	E	26	ALA	2.5
1	E	209	ASP	2.5
1	E	410	MET	2.5
1	H	154	VAL	2.5
1	E	448	ASN	2.5
1	H	131	LEU	2.5
1	E	236	GLU	2.5
1	E	71	GLY	2.5
1	G	415	SER	2.5
1	C	318	THR	2.5
1	F	348	ASP	2.5
1	D	68	ALA	2.5
1	G	328	VAL	2.5
1	G	410	MET	2.5
1	H	439	LEU	2.5
1	C	114	HIS	2.5
1	A	216	GLU	2.5
1	B	373	GLU	2.5
1	G	241	GLY	2.5
1	C	443	ILE	2.5
1	F	136	VAL	2.5
1	D	392	TRP	2.4
1	B	87	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	2.4
1	G	169	THR	2.4
1	C	225	LEU	2.4
1	F	155	VAL	2.4
1	D	202	LYS	2.4
1	D	335	GLU	2.4
1	G	404	PRO	2.4
1	E	205	GLY	2.4
1	B	203	ASN	2.4
1	G	28	LEU	2.4
1	G	326	ASP	2.4
1	B	279	SER	2.4
1	G	242	ILE	2.4
1	G	413	ILE	2.4
1	D	449	TYR	2.4
1	E	217	ASN	2.4
1	C	279	SER	2.4
1	G	240	ILE	2.4
1	E	107	LYS	2.4
1	G	187	MET	2.4
1	E	82	GLU	2.4
1	E	66	GLY	2.4
1	B	181	GLU	2.4
1	G	87	LYS	2.4
1	C	297	THR	2.4
1	G	225	LEU	2.4
1	E	291	ARG	2.4
1	B	441	GLN	2.4
1	H	112	GLY	2.4
1	A	114	HIS	2.4
1	E	195	GLU	2.4
1	E	172	SER	2.4
1	A	115	LEU	2.4
1	B	51	ARG	2.4
1	F	279	SER	2.4
1	E	444	ILE	2.3
1	G	232	ILE	2.3
1	B	380	PHE	2.3
1	A	151	VAL	2.3
1	E	80	GLU	2.3
1	B	366	ASN	2.3
1	E	440	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	107	LYS	2.3
1	H	150	ASP	2.3
1	B	206	TYR	2.3
1	D	278	SER	2.3
1	F	454	GLY	2.3
1	F	153	VAL	2.3
1	G	405	HIS	2.3
1	D	237	ASN	2.3
1	G	429	PRO	2.3
1	A	409	SER	2.3
1	D	83	SER	2.3
1	F	299	GLY	2.3
1	C	111	THR	2.3
1	C	440	LEU	2.3
1	E	346	ILE	2.3
1	G	174	TRP	2.3
1	A	300	ILE	2.3
1	G	372	ILE	2.3
1	G	434	ASN	2.3
1	G	115	LEU	2.3
1	B	381	ALA	2.2
1	B	114	HIS	2.2
1	E	222	HIS	2.2
1	E	143	ASN	2.2
1	E	407	PRO	2.2
1	B	129	GLY	2.2
1	D	129	GLY	2.2
1	A	440	LEU	2.2
1	E	40	LEU	2.2
1	E	49	VAL	2.2
1	G	212	ALA	2.2
1	B	191	GLU	2.2
1	D	386	ASP	2.2
1	A	319	LEU	2.2
1	B	187	MET	2.2
1	D	275	LEU	2.2
1	F	275	LEU	2.2
1	E	373	GLU	2.2
1	H	191	GLU	2.2
1	G	202	LYS	2.2
1	D	209	ASP	2.2
1	A	297	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	317	PHE	2.2
1	H	436	PHE	2.2
1	E	225	LEU	2.2
1	H	128	LEU	2.2
1	D	216	GLU	2.2
1	E	144	ASN	2.2
1	G	68	ALA	2.2
1	G	182	GLU	2.2
1	G	203	ASN	2.2
1	D	106	GLY	2.2
1	D	138	ARG	2.2
1	H	225	LEU	2.2
1	A	191	GLU	2.2
1	A	109	THR	2.2
1	B	148	ASN	2.2
1	H	297	THR	2.2
1	A	315	VAL	2.2
1	B	88	VAL	2.2
1	D	194	PRO	2.2
1	E	37	GLN	2.2
1	H	54	GLN	2.2
1	B	291	ARG	2.2
1	D	51	ARG	2.2
1	G	450	ARG	2.2
1	E	122	GLY	2.1
1	E	387	GLN	2.1
1	G	226	HIS	2.1
1	H	155	VAL	2.1
1	A	301	ILE	2.1
1	G	147	PRO	2.1
1	G	211	PRO	2.1
1	H	113	SER	2.1
1	F	296	PHE	2.1
1	D	348	ASP	2.1
1	G	220	ASP	2.1
1	E	64	LEU	2.1
1	B	210	THR	2.1
1	B	449	TYR	2.1
1	F	223	PHE	2.1
1	G	80	GLU	2.1
1	E	275	LEU	2.1
1	E	78	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	114	HIS	2.1
1	B	215	LYS	2.1
1	C	110	ALA	2.1
1	E	31	ALA	2.1
1	F	375	VAL	2.1
1	A	432	ILE	2.1
1	A	134	LEU	2.1
1	H	115	LEU	2.1
1	G	445	ASN	2.1
1	D	385	LYS	2.1
1	H	86	CYS	2.1
1	D	147	PRO	2.1
1	A	444	ILE	2.1
1	H	223	PHE	2.1
1	B	190	GLY	2.1
1	D	60	GLY	2.1
1	H	152	CYS	2.1
1	H	215	LYS	2.1
1	G	250	ASN	2.1
1	G	294	GLY	2.1
1	H	222	HIS	2.1
1	A	438	VAL	2.1
1	G	409	SER	2.1
1	D	182	GLU	2.1
1	G	47	GLY	2.1
1	A	19	THR	2.1
1	G	397	HIS	2.1
1	A	136	VAL	2.1
1	A	316	SER	2.1
1	B	274	ALA	2.1
1	C	316	SER	2.1
1	E	395	ALA	2.1
1	G	165	ALA	2.1
1	G	238	LYS	2.1
1	H	110	ALA	2.1
1	F	151	VAL	2.1
1	F	278	SER	2.1
1	E	51	ARG	2.1
1	E	383	PHE	2.1
1	G	180	LEU	2.1
1	H	193	LYS	2.0
1	G	38	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	109	THR	2.0
1	H	318	THR	2.0
1	H	331	THR	2.0
1	B	23	PRO	2.0
1	E	274	ALA	2.0
1	G	351	ALA	2.0
1	G	376	SER	2.0
1	B	120	GLU	2.0
1	C	216	GLU	2.0
1	G	61	MET	2.0
1	B	126	GLY	2.0
1	C	409	SER	2.0
1	G	121	ALA	2.0
1	G	154	VAL	2.0
1	H	419	LEU	2.0
1	E	441	GLN	2.0
1	E	74	ARG	2.0
1	B	312	PRO	2.0
1	D	162	ALA	2.0
1	E	378	SER	2.0
1	H	409	SER	2.0
1	G	401	GLN	2.0
1	E	202	LYS	2.0
1	E	417	ASP	2.0
1	H	327	ASP	2.0
1	H	408	THR	2.0
1	B	370	VAL	2.0
1	E	406	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	BIB	E	6502	7/7	0.28	4.79	21,22,24,24	0
3	BIB	G	8502	7/7	0.30	3.20	19,21,21,22	0
3	BIB	C	3502	7/7	0.26	2.40	24,26,27,27	0
3	BIB	E	5502	7/7	0.30	1.58	16,17,18,18	0
3	BIB	D	4502	7/7	0.22	0.27	16,16,17,17	0
3	BIB	G	7502	7/7	0.34	0.24	12,13,15,15	0
3	BIB	A	2502	7/7	0.20	0.09	15,19,21,21	0
3	BIB	B	1502	7/7	0.21	-0.60	19,23,24,25	0
2	ZN	A	500	1/1	0.21	-0.72	15,15,15,15	0
2	ZN	F	500	1/1	0.18	-1.01	16,16,16,16	0
2	ZN	C	500	1/1	0.18	-1.06	16,16,16,16	0
2	ZN	H	500	1/1	0.15	-1.40	15,15,15,15	0
2	ZN	C	501	1/1	0.14	-1.42	18,18,18,18	0
2	ZN	B	500	1/1	0.12	-1.70	16,16,16,16	0
2	ZN	A	501	1/1	0.15	-1.71	18,18,18,18	0
2	ZN	F	501	1/1	0.13	-1.77	18,18,18,18	0
2	ZN	H	501	1/1	0.13	-1.90	18,18,18,18	0
2	ZN	G	501	1/1	0.14	-2.36	17,17,17,17	0
2	ZN	E	500	1/1	0.07	-2.48	16,16,16,16	0
2	ZN	B	501	1/1	0.05	-2.89	18,18,18,18	0
2	ZN	D	500	1/1	0.08	-2.92	15,15,15,15	0
2	ZN	G	500	1/1	0.06	-3.02	15,15,15,15	0
2	ZN	D	501	1/1	0.07	-3.65	18,18,18,18	0
2	ZN	E	501	1/1	0.08	-3.74	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.