Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 12:09 PM EST

PDB ID	:	1R3N
Title	:	Crystal structure of beta-alanine synthase from Saccharomyces kluyveri
Authors	:	Lundgren, S.; Gojkovic, Z.; Piskur, J.; Dobritzsch, D.
Deposited on	:	2003-10-02
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

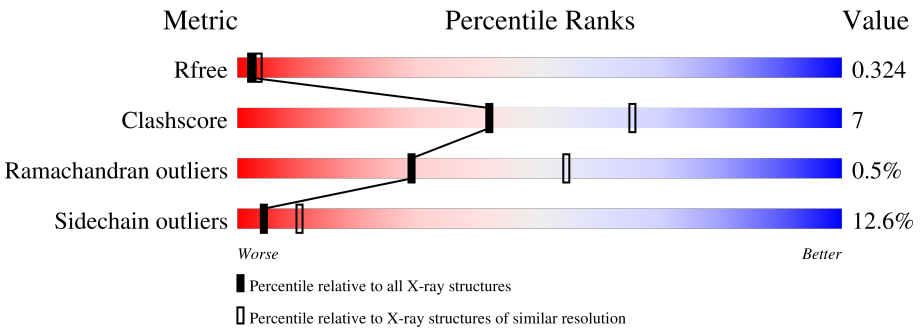
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	462	73% 19% • 5%
1	B	462	71% 21% • 6%
1	C	462	76% 16% • 5%
1	D	462	75% 17% • 5%
1	E	462	64% 26% 5% 6%
1	F	462	76% 16% • 5%
1	G	462	65% 24% • 7%

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Mol	Chain	Length	Quality of chain
1	H	462	73% 19% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27487 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 beta-alanine synthase.

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

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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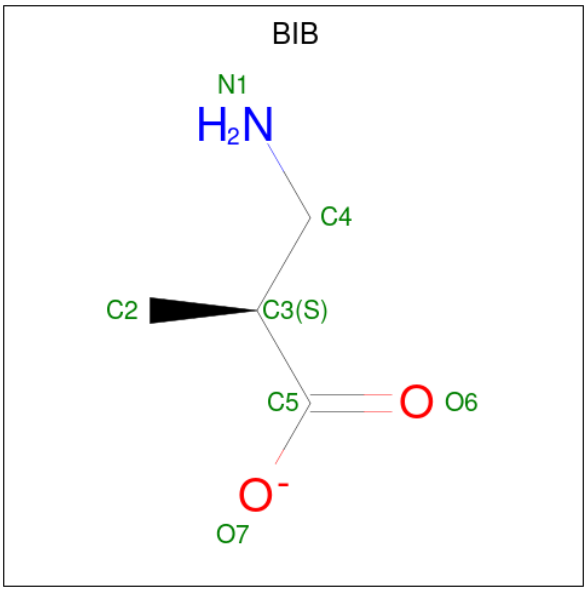
Chain	Residue	Modelled	Actual	Comment	Reference
G	463	HIS	-	expression tag	UNP Q96W94
H	456	HIS	-	expression tag	UNP Q96W94
H	457	HIS	-	expression tag	UNP Q96W94
H	458	HIS	-	expression tag	UNP Q96W94
H	459	HIS	-	expression tag	UNP Q96W94
H	460	HIS	-	expression tag	UNP Q96W94
H	461	HIS	-	expression tag	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
			Total	Zn		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0
2	E	2	2	2	0	0
2	F	2	2	2	0	0
2	G	2	2	2	0	0
2	H	2	2	2	0	0

- Molecule 3 is BETA-AMINO ISOBUTYRATE (three-letter code: BIB) (formula: $C_4H_8NO_2$).



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

- Molecule 4 is water.

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

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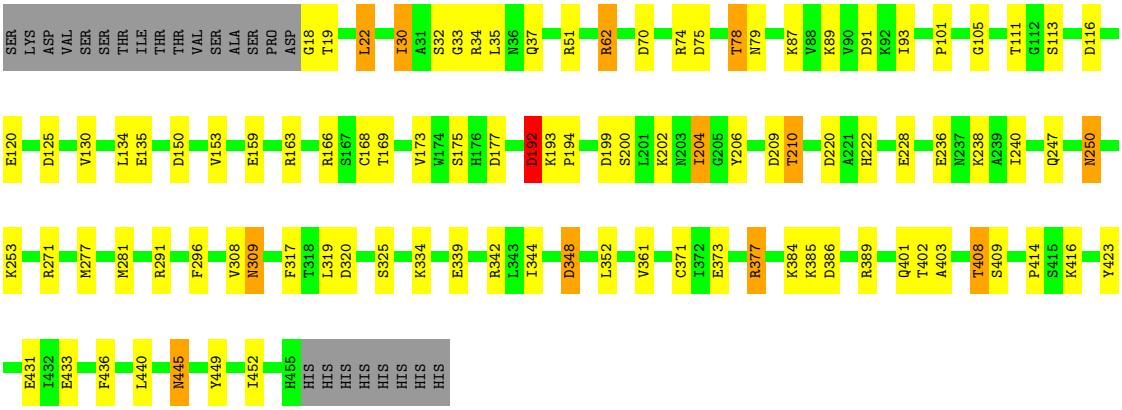
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	20	20	20	0	0
			Total	O		
4	F	101	101	101	0	0
			Total	O		
4	G	24	24	24	0	0
			Total	O		
4	H	50	50	50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

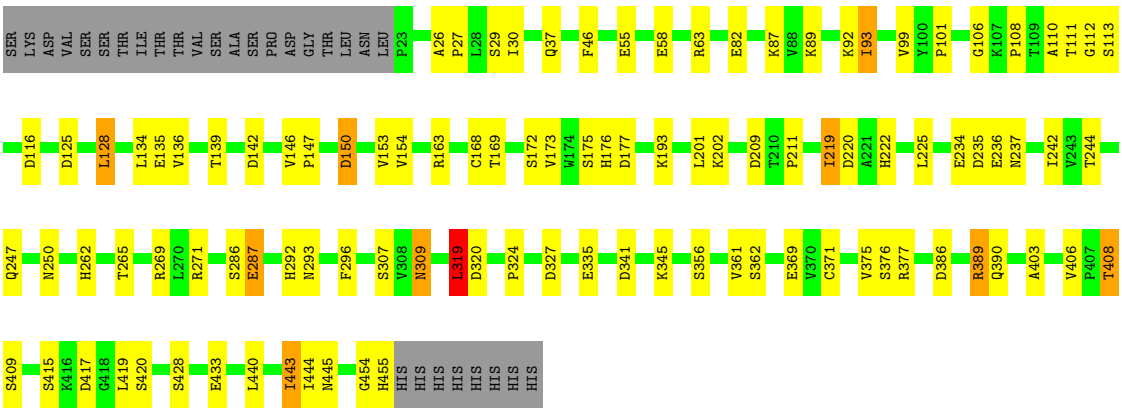
- Molecule 1: beta-alanine synthase

Chain A:



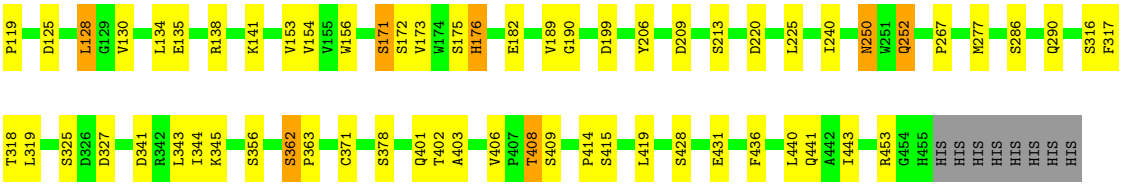
- Molecule 1: beta-alanine synthase

Chain B:



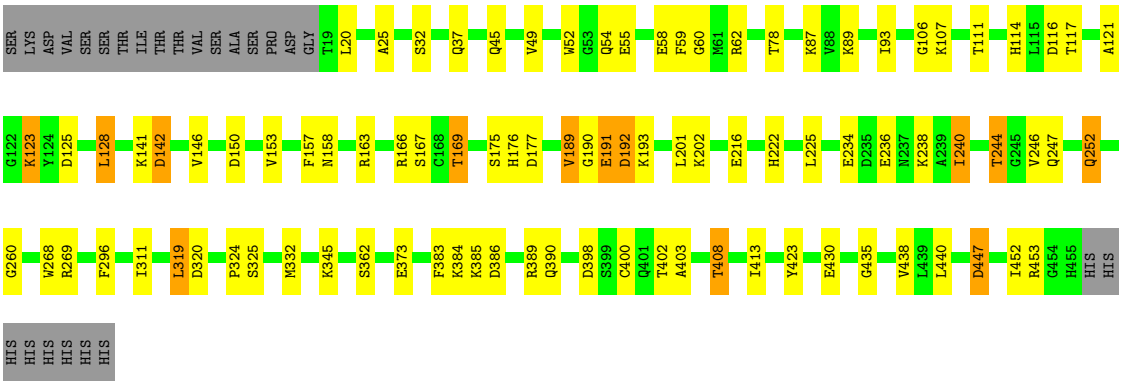
- Molecule 1: beta-alanine synthase

Chain C:



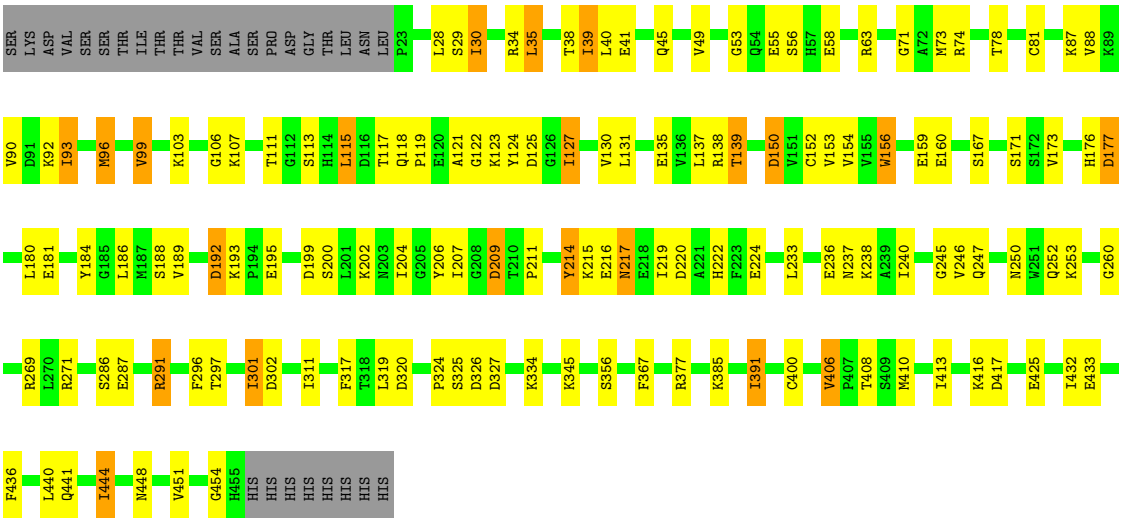
- Molecule 1: beta-alanine synthase

Chain D:



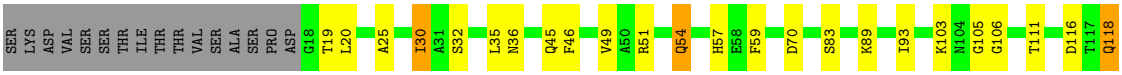
- Molecule 1: beta-alanine synthase

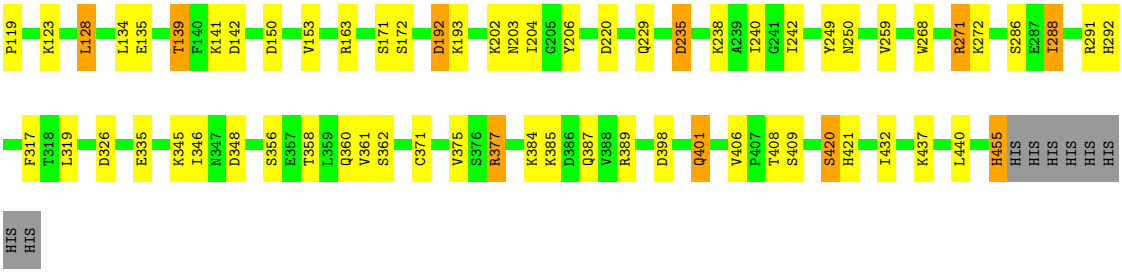
Chain E:



- Molecule 1: beta-alanine synthase

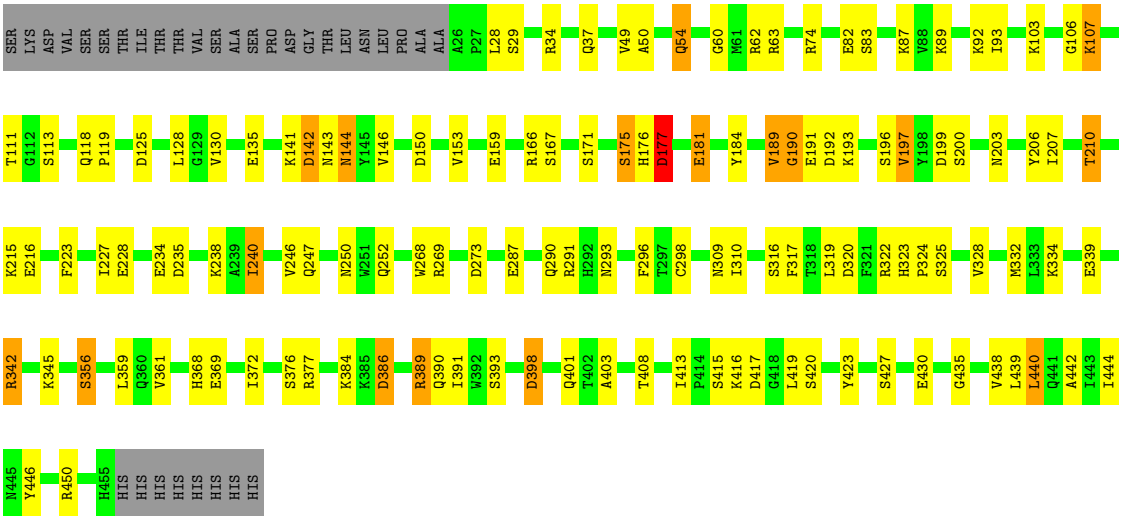
Chain F:





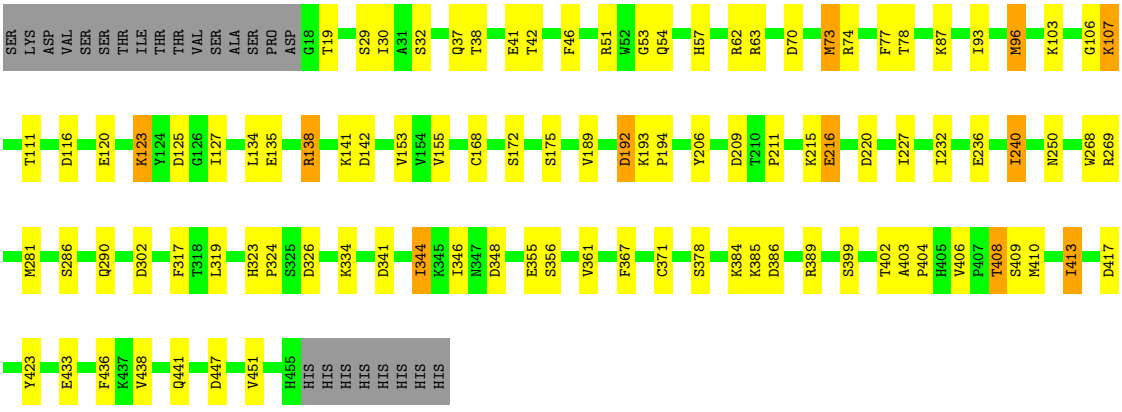
- Molecule 1: beta-alanine synthase

Chain G:



- Molecule 1: beta-alanine synthase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	5296 reflections (4.99%)	wwPDB-VP
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 , 19.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 (370) 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: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
1:H:346:ILE:HD11	4:H:511:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:F:455:HIS:CD2	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:A:371:CYS:HB3	1:A:409:SER:HB2	1.77	0.67
1:D:189:VAL:CG2	1:D:190:GLY:H	2.06	0.67
1:E:269:ARG:NH2	1:F:235:ASP:OD1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:C:182:GLU:OE1	4:C:3559:HOH:O	2.12	0.66
1:D:244:THR:O	4:D:4531:HOH:O	2.14	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:HG13	1:E:88:VAL:O	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:E:63:ARG:HH12	1:E:115:LEU:HB3	1.65	0.60
1:F:118:GLN:HG3	1:F:119:PRO:HD3	1.82	0.60
1:E:118:GLN:HG3	1:E:119:PRO:CD	2.24	0.60
1:C:128:LEU:HD13	1:C:225:LEU:HG	1.83	0.60
1:E:30:ILE:HG21	1:E:436:PHE:HE2	1.66	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:E:317:PHE:CE1	1:E:319:LEU:HD21	2.38	0.59
1:F:25:ALA:O	4:F:576:HOH:O	2.17	0.59
1:B:128:LEU:HD13	1:B:225:LEU:HG	1.83	0.59
1:D:413:ILE:HD11	1:D:435:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ARG:HB3	1:E:206:TYR:CZ	2.38	0.58
1:H:120:GLU:HG2	1:H:423:TYR:CZ	2.39	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:367:PHE:CE2	1:H:410:MET:HG3	2.38	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:D:60:GLY:HA3	1:D:423:TYR:CD2	2.38	0.58
1:E:35:LEU:HD12	1:E:436:PHE:HB2	1.85	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:A:62:ARG:HD3	4:A:2609:HOH:O	2.04	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:C:277:MET:HE1	1:C:343:LEU:O	2.04	0.57
1:G:159:GLU:OE1	4:G:8505:HOH:O	2.17	0.57
1:H:134:LEU:HG	1:H:138:ARG:HD2	1.85	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:HG23	1:H:19:THR:O	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:HB2	1:E:291:ARG:HH11	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:A:414:PRO:HD2	1:A:431:GLU:HG2	1.90	0.54
1:B:175:SER:O	1:B:176:HIS:HB2	2.07	0.54
1:A:101:PRO:HA	1:A:150:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:GLU:HG2	4:A:2564:HOH:O	2.07	0.53
1:C:371:CYS:HB3	1:C:409:SER:CB	2.38	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:G:247:GLN:HE21	1:G:324:PRO:HD3	1.74	0.52
1:H:371:CYS:CB	1:H:409:SER:HB2	2.40	0.52
1:E:233:LEU:HD22	1:E:238:LYS:HB2	1.91	0.52
1:C:317:PHE:HE1	1:C:319:LEU:HD21	1.74	0.52
1:F:35:LEU:HB2	1:F:135:GLU:HG3	1.92	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:G:317:PHE:HE1	1:G:319:LEU:HD21	1.74	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:A:403:ALA:HA	1:A:408:THR:HG23	1.93	0.51
1:G:175:SER:OG	1:G:401:GLN:O	2.27	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:D:114:HIS:HB2	1:D:116:ASP:OD1	2.11	0.50
1:D:240:ILE:HG12	1:D:438:VAL:HG21	1.92	0.50
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:G:166:ARG:HG3	1:G:166:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:20:LEU:O	1:F:377:ARG:NH1	2.43	0.50
1:G:413:ILE:HD11	1:G:435:GLY:HA2	1.92	0.50
1:D:166:ARG:O	1:D:169:THR:HG22	2.10	0.50
1:D:238:LYS:HD2	1:D:389:ARG:HB2	1.92	0.50
1:G:171:SER:O	1:G:175:SER:HB2	2.11	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:B:92:LYS:HD2	1:B:211:PRO:HA	1.94	0.49
1:C:267:PRO:HB2	4:C:3548:HOH:O	2.11	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: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:238:LYS:HD2	1:G:389:ARG:HB2	1.94	0.49
1:B:26:ALA:HB2	1:G:291:ARG:O	2.13	0.49
1:B:169:THR:O	1:B:173:VAL:HG13	2.11	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:C:378:SER:OG	1:C:441:GLN:HB3	2.11	0.49
1:E:34:ARG:CZ	1:E:138:ARG:HD2	2.42	0.49
1:A:222:HIS:O	1:A:408:THR:HB	2.13	0.48
1:E:214:TYR:HD1	1:E:214:TYR:H	1.61	0.48
1:E:233:LEU:HD21	1:E:391:ILE:HD11	1.94	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:HG2	1:D:269:ARG:HH11	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:A:159:GLU:HG2	1:A:168:CYS:SG	2.54	0.47
1:F:249:TYR:CE2	1:F:362:SER:HB3	2.49	0.47
1:G:111:THR:O	1:G:153:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HG2	1:A:135:GLU:OE1	2.13	0.47
1:E:115:LEU:HD21	1:E:130:VAL:HG21	1.96	0.47
1:H:57:HIS:O	1:H:123:LYS:HE2	2.15	0.47
1:A:33:GLY:O	1:A:37:GLN:HG2	2.14	0.47
1:A:402:THR:OG1	1:A:408:THR:HG21	2.15	0.47
1:E:122:GLY:HA3	1:E:425:GLU:HB3	1.96	0.47
1:B:287:GLU:HG3	4:B:1549:HOH:O	2.15	0.47
1:H:240:ILE:HG12	1:H:438:VAL:HG21	1.96	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:A:250:ASN:C	1:A:250:ASN:HD22	2.18	0.46
1:E:317:PHE:HE1	1:E:319:LEU:HD21	1.77	0.46
1:F:249:TYR:OH	1:F:360:GLN:NE2	2.47	0.46
1:G:60:GLY:HA3	1:G:423:TYR:CD2	2.50	0.46
1:H:402:THR:OG1	1:H:408:THR:HG21	2.16	0.46
1:A:18:GLY:HA2	1:A:22:LEU:HD13	1.96	0.46
1:E:30:ILE:HG21	1:E:436:PHE:CE2	2.49	0.46
1:E:78:THR:CG2	1:E:88:VAL:HG11	2.35	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:B:406:VAL:HG23	1:B:408:THR:HG22	1.97	0.46
1:F:259:VAL:HG23	1:F:272:LYS:HD2	1.98	0.46
1:B:111:THR:O	1:B:153:VAL:HA	2.17	0.45
1:B:234:GLU:OE2	1:B:417:ASP:N	2.46	0.45
1:C:100:TYR:HA	1:C:101:PRO:HD3	1.81	0.45
1:C:406:VAL:HG23	1:C:408:THR:HG22	1.97	0.45
1:E:74:ARG:HB3	1:E:206:TYR:OH	2.16	0.45
1:C:74:ARG:HB3	1:C:206:TYR:CZ	2.51	0.45
1:E:38:THR:HG21	1:E:138:ARG:HH22	1.81	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:A:281:MET:HE3	1:A:344:ILE:HD13	1.98	0.45
1:B:292:HIS:HE1	1:B:335:GLU:OE1	2.00	0.45
1:C:171:SER:O	1:C:175:SER:HB2	2.16	0.45
1:F:36:ASN:ND2	1:F:432:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:CYS:O	1:H:172:SER:OG	2.32	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
1:A:377:ARG:HD3	1:A:377:ARG:HA	1.76	0.45
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: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:O	1:H:30:ILE:HG13	2.17	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:D:246:VAL:HG21	1:D:400:CYS:SG	2.57	0.44
1:D:157:PHE:CE1	1:D:201:LEU:HD21	2.52	0.44
1:F:45:GLN:HG2	1:F:46:PHE:CE1	2.52	0.44
1:F:128:LEU:HD21	1:F:432:ILE:HG23	1.99	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:E:245:GLY:HA2	1:E:367:PHE:CD1	2.53	0.44
1:G:310:ILE:HD12	4:G:8520:HOH:O	2.18	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:281:MET:CE	1:H:344:ILE:HG23	2.48	0.43
1:H:317:PHE:HE1	1:H:319:LEU:HD21	1.80	0.43
1:D:111:THR:O	1:D:153:VAL:HA	2.19	0.43
1:G:323:HIS:ND1	1:G:324:PRO:HD2	2.33	0.43
1:H:107:LYS:H	1:H:107:LYS:HG3	1.55	0.43
1:C:73:MET:CE	1:C:115:LEU:HD22	2.49	0.43
1:E:99:VAL:O	1:E:99:VAL:HG12	2.18	0.43
1:H:120:GLU:HG2	1:H:423:TYR:CE2	2.54	0.43
1:B:93:ILE:O	1:B:93:ILE:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:O	1:A:173:VAL:HG23	2.19	0.43
1:C:113:SER:HB3	1:C:130:VAL:HG23	1.99	0.43
1:A:177:ASP:OD2	1:A:401:GLN:NE2	2.52	0.43
1:B:222:HIS:O	1:B:408:THR:HB	2.19	0.43
1:C:406:VAL:O	1:C:408:THR:HG23	2.19	0.43
1:E:117:THR:HB	1:E:121:ALA:CB	2.49	0.43
1:G:107:LYS:O	1:G:450:ARG:NH2	2.50	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:A:89:LYS:CD	1:A:210:THR:HG21	2.49	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: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:G:247:GLN:NE2	1:G:324:PRO:HD3	2.33	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:B:168:CYS:O	1:B:172:SER:HB2	2.20	0.42
1:D:252:GLN:HB2	4:D:4554:HOH:O	2.20	0.42
1:E:124:TYR:CD2	1:E:432:ILE:HD11	2.55	0.42
1:E:271:ARG:CZ	1:E:311:ILE:HD11	2.50	0.42
1:H:371:CYS:HB2	1:H:409:SER:HB2	2.02	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:A:30:ILE:HD11	1:A:440:LEU:HD22	2.01	0.42
1:C:63:ARG:HB3	1:C:117:THR:HG23	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:C:362:SER:HA	1:C:363:PRO:HD3	1.79	0.42
1:F:288:ILE:HG13	1:F:291:ARG:NH2	2.34	0.42
1:C:414:PRO:HG2	1:C:431:GLU:CD	2.39	0.42
1:F:172:SER:HA	1:F:401:GLN:HG3	2.02	0.42
1:H:378:SER:OG	1:H:441:GLN:HB3	2.19	0.42
1:C:111:THR:O	1:C:153:VAL:HA	2.19	0.42
1:E:93:ILE:HG23	1:E:93:ILE:O	2.20	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:C:402:THR:OG1	1:C:408:THR:HG21	2.20	0.41
1:D:189:VAL:CG2	1:D:190:GLY:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:CYS:SG	1:G:317:PHE:HB2	2.60	0.41
1:B:403:ALA:HA	1:B:408:THR:HG23	2.02	0.41
1:C:290:GLN:HG2	1:D:268:TRP:CE2	2.55	0.41
1:E:127:ILE:H	1:E:127:ILE:HG12	1.53	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:D:402:THR:OG1	1:D:408:THR:HG21	2.20	0.41
1:G:339:GLU:OE2	1:G:342:ARG:NH1	2.52	0.41
1:G:398:ASP:OD1	1:G:398:ASP:N	2.44	0.41
1:H:74:ARG:HB3	1:H:206:TYR:CZ	2.56	0.41
1:H:127:ILE:H	1:H:127:ILE:HG12	1.62	0.41
1:B:319:LEU:N	1:B:319:LEU:HD23	2.36	0.41
1:C:78:THR:HB	1:C:88:VAL:HG11	2.01	0.41
1:A:22:LEU:HD11	1:A:449:TYR:HB2	2.02	0.41
1:A:111:THR:O	1:A:153:VAL:HA	2.21	0.41
1:B:242:ILE:HD12	1:B:375:VAL:HG12	2.02	0.41
1:B:443:ILE:H	1:B:443:ILE:HG12	1.71	0.41
1:G:181:GLU:H	1:G:181:GLU:HG3	1.57	0.41
1:H:192:ASP:O	1:H:194:PRO:HD3	2.21	0.41
1:B:146:VAL:HA	1:B:147:PRO:HD3	1.90	0.41
1:E:38:THR:HG21	1:E:138:ARG:NH2	2.36	0.41
1:E:224:GLU:HB3	1:E:410:MET:HG2	2.03	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:54:GLN:HE21	1:G:54:GLN:HB3	1.70	0.41
1:G:223:PHE:CE2	1:G:442:ALA:HB1	2.56	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:A:238:LYS:HD3	1:A:386:ASP:O	2.21	0.40
1:B:46:PHE:O	1:B:63:ARG:HD3	2.21	0.40
1:B:361:VAL:N	4:B:1525:HOH:O	2.49	0.40
1:E:38:THR:HA	1:E:41:GLU:HG2	2.02	0.40
1:E:125:ASP:O	1:E:127:ILE:HG12	2.22	0.40
1:H:77:PHE:CD2	1:H:96:MET:CE	3.04	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	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:ND2	1:G:144:ASN:O[1_565]	1.98	0.22

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/462 (94%)	420 (96%)	16 (4%)	0	100	100
1	B	431/462 (93%)	418 (97%)	11 (3%)	2 (0%)	29	54
1	C	436/462 (94%)	420 (96%)	14 (3%)	2 (0%)	29	54
1	D	435/462 (94%)	419 (96%)	12 (3%)	4 (1%)	17	40
1	E	431/462 (93%)	417 (97%)	12 (3%)	2 (0%)	29	54
1	F	436/462 (94%)	422 (97%)	12 (3%)	2 (0%)	29	54
1	G	428/462 (93%)	411 (96%)	13 (3%)	4 (1%)	17	40
1	H	436/462 (94%)	422 (97%)	13 (3%)	1 (0%)	47	73
All	All	3469/3696 (94%)	3349 (96%)	103 (3%)	17 (0%)	29	54

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	360/383 (94%)	323 (90%)	37 (10%)	7 16
1	B	356/383 (93%)	314 (88%)	42 (12%)	5 12
1	C	360/383 (94%)	332 (92%)	28 (8%)	12 29
1	D	360/383 (94%)	317 (88%)	43 (12%)	5 12
1	E	356/383 (93%)	284 (80%)	72 (20%)	1 3
1	F	360/383 (94%)	321 (89%)	39 (11%)	6 15
1	G	355/383 (93%)	289 (81%)	66 (19%)	1 4
1	H	360/383 (94%)	325 (90%)	35 (10%)	8 19
All	All	2867/3064 (94%)	2505 (87%)	362 (13%)	4 10

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

Sometimes 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

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Mol	Chain	Res	Type
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
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	G	8502	-	5,6,6	1.00	0	4,7,7	1.04	0
3	BIB	G	7502	-	5,6,6	0.90	0	4,7,7	0.93	0
3	BIB	B	1502	-	5,6,6	1.02	0	4,7,7	1.20	0
3	BIB	A	2502	-	5,6,6	0.99	0	4,7,7	0.79	0
3	BIB	D	4502	-	5,6,6	0.98	0	4,7,7	0.92	0
3	BIB	E	6502	-	5,6,6	0.87	0	4,7,7	1.19	0
3	BIB	C	3502	-	5,6,6	1.01	0	4,7,7	1.05	0
3	BIB	E	5502	-	5,6,6	1.01	0	4,7,7	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BIB	G	8502	-	-	0/5/6/6	-
3	BIB	G	7502	-	-	0/5/6/6	-
3	BIB	B	1502	-	-	1/5/6/6	-
3	BIB	A	2502	-	-	0/5/6/6	-
3	BIB	D	4502	-	-	0/5/6/6	-
3	BIB	E	6502	-	-	2/5/6/6	-
3	BIB	C	3502	-	-	0/5/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BIB	E	5502	-	-	0/5/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	6502	BIB	C4-C3-C5-O7
3	E	6502	BIB	C4-C3-C5-O6
3	B	1502	BIB	C2-C3-C4-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2502	BIB	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.