Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:29 AM GMT

PDB ID	:	2QUY
Title	:	Truncated mutant ASN175ALA of penicillin v acylase from bacillus sphaericus
Authors	:	Pathak, M.C.; Brannigan, J.; Dodson, G.G.; Suresh, C.G.
Deposited on	:	2007-08-07
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

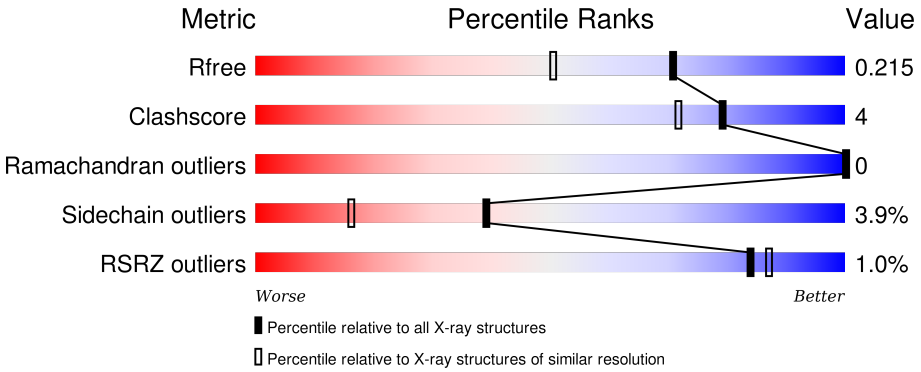
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	86% 11%
1	B	335	89% 9%
1	C	335	86% 11%
1	D	335	87% 9%
1	E	335	85% 13%

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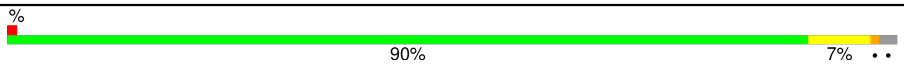
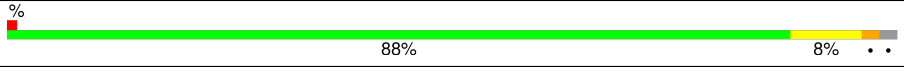
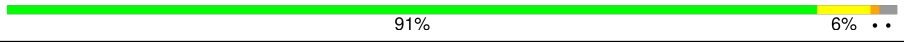
Mol	Chain	Length	Quality of chain
1	F	335	
1	G	335	
1	H	335	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21995 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 Penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2576	1640	422	501	13			
1	B	330	Total	C	N	O	S	0	0	0
			2576	1640	422	501	13			
1	C	330	Total	C	N	O	S	0	0	0
			2576	1640	422	501	13			
1	D	330	Total	C	N	O	S	0	0	0
			2576	1640	422	501	13			
1	E	330	Total	C	N	O	S	0	1	0
			2579	1641	423	502	13			
1	F	329	Total	C	N	O	S	0	0	0
			2567	1635	420	499	13			
1	G	329	Total	C	N	O	S	0	0	0
			2567	1635	420	499	13			
1	H	329	Total	C	N	O	S	0	0	0
			2567	1635	420	499	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ARG	THR	CONFLICT	UNP P12256
A	175	ALA	ASN	ENGINEERED	UNP P12256
B	98	ARG	THR	CONFLICT	UNP P12256
B	175	ALA	ASN	ENGINEERED	UNP P12256
C	98	ARG	THR	CONFLICT	UNP P12256
C	175	ALA	ASN	ENGINEERED	UNP P12256
D	98	ARG	THR	CONFLICT	UNP P12256
D	175	ALA	ASN	ENGINEERED	UNP P12256
E	98	ARG	THR	CONFLICT	UNP P12256
E	175	ALA	ASN	ENGINEERED	UNP P12256
F	98	ARG	THR	CONFLICT	UNP P12256
F	175	ALA	ASN	ENGINEERED	UNP P12256
G	98	ARG	THR	CONFLICT	UNP P12256

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Chain	Residue	Modelled	Actual	Comment	Reference
G	175	ALA	ASN	ENGINEERED	UNP P12256
H	98	ARG	THR	CONFLICT	UNP P12256
H	175	ALA	ASN	ENGINEERED	UNP P12256

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	E	2	Total Cl 2 2	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is water.

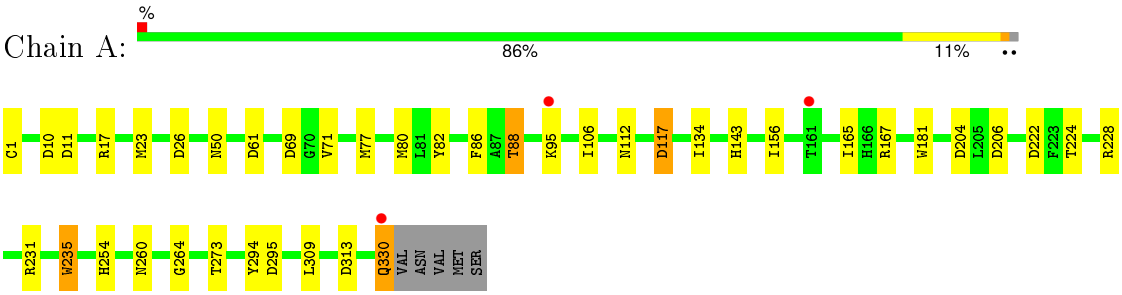
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	193	Total O 193 193	0	0
3	B	185	Total O 185 185	0	0
3	C	163	Total O 163 163	0	0
3	D	164	Total O 164 164	0	0
3	E	186	Total O 186 186	0	0
3	F	165	Total O 165 165	0	0
3	G	154	Total O 154 154	0	0
3	H	193	Total O 193 193	0	0

3 Residue-property plots (i)

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

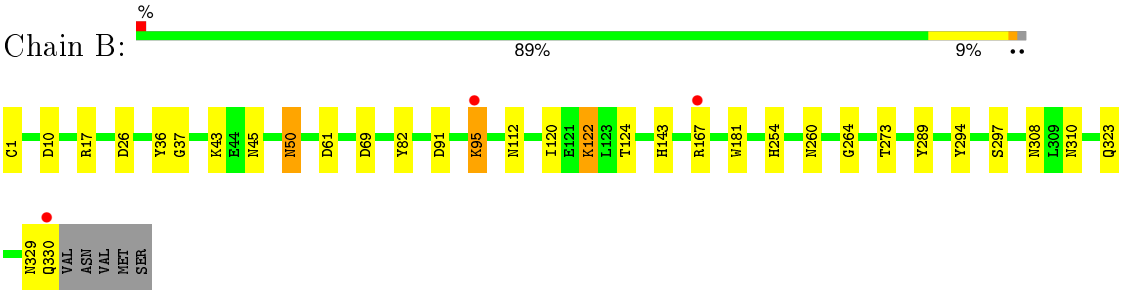
- Molecule 1: Penicillin acylase

Chain A:



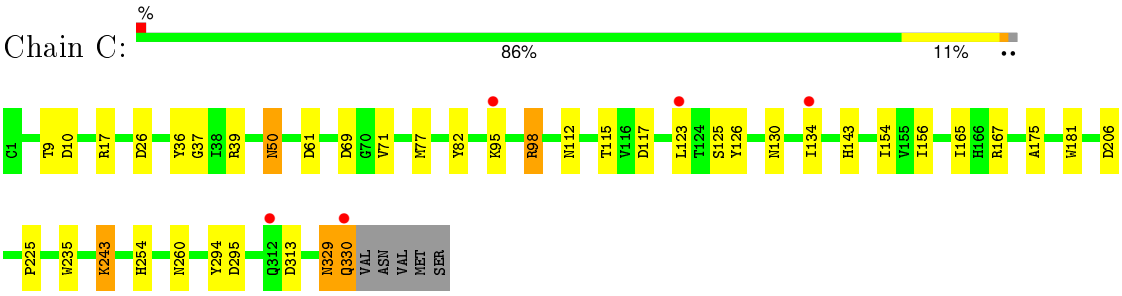
- Molecule 1: Penicillin acylase

Chain B:



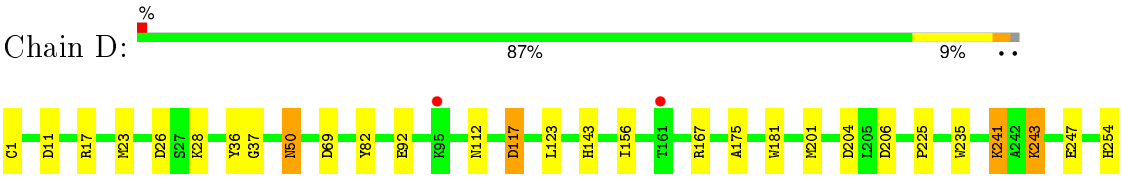
- Molecule 1: Penicillin acylase

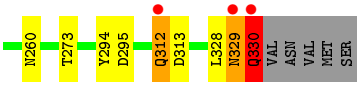
Chain C:



- Molecule 1: Penicillin acylase

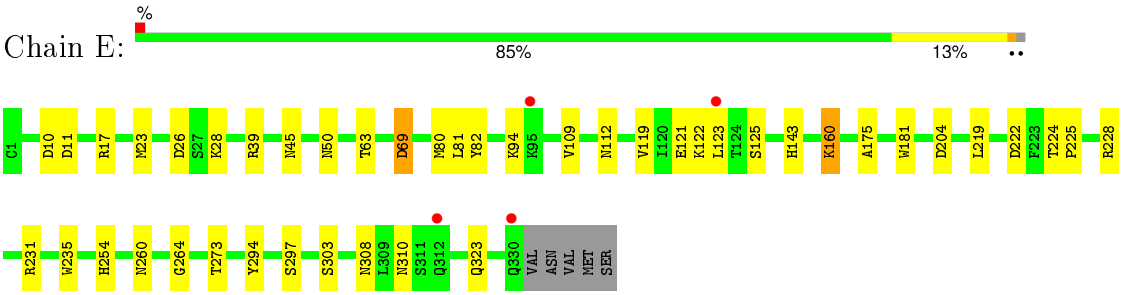
Chain D:





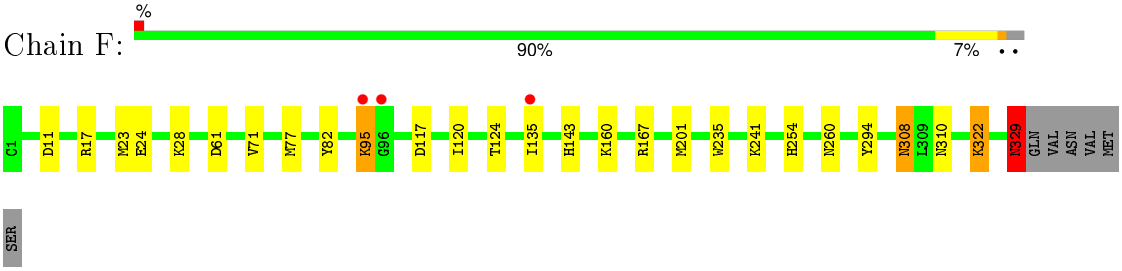
• Molecule 1: Penicillin acylase

Chain E:



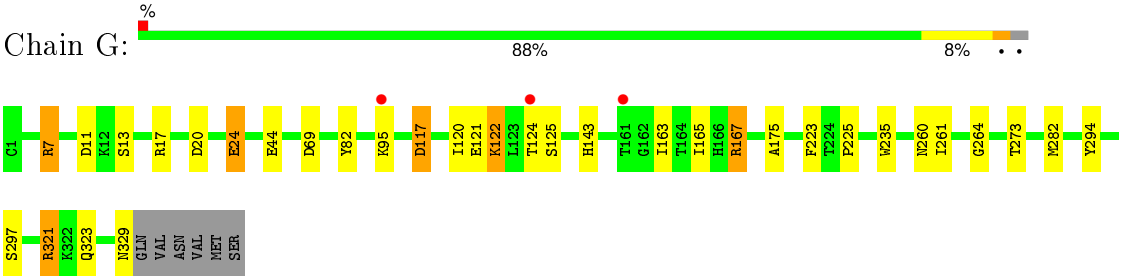
• Molecule 1: Penicillin acylase

Chain F:



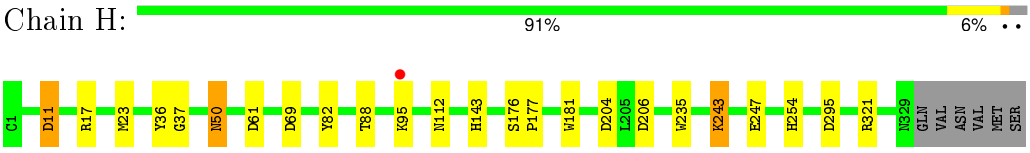
• Molecule 1: Penicillin acylase

Chain G:



• Molecule 1: Penicillin acylase

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	47.29Å 379.38Å 102.01Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 47.23 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-1.70) 94.2 (47.23-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.175 , 0.203 0.190 , 0.215	Depositor DCC
R_{free} test set	18580 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	2 of 370593 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21995	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.84	1/2631 (0.0%)	1.00	16/3576 (0.4%)
1	B	0.88	2/2631 (0.1%)	0.96	7/3576 (0.2%)
1	C	0.85	0/2631	0.99	16/3576 (0.4%)
1	D	0.82	0/2631	0.95	11/3576 (0.3%)
1	E	0.83	0/2639	0.93	6/3587 (0.2%)
1	F	0.85	2/2622 (0.1%)	0.92	3/3564 (0.1%)
1	G	0.83	1/2622 (0.0%)	0.90	5/3564 (0.1%)
1	H	0.82	0/2622	0.95	6/3564 (0.2%)
All	All	0.84	6/21029 (0.0%)	0.95	70/28583 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	329	ASN	C-O	-9.12	1.06	1.23
1	B	329	ASN	C-O	9.07	1.40	1.23
1	G	329	ASN	C-O	-8.03	1.08	1.23
1	A	235	TRP	CB-CG	5.33	1.59	1.50
1	B	289	TYR	CD2-CE2	5.32	1.47	1.39
1	F	201	MET	CG-SD	-5.08	1.68	1.81

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	GLN	N-CA-CB	-11.43	90.03	110.60
1	C	39	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	61	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	69	ASP	CB-CG-OD2	7.93	125.44	118.30
1	D	329	ASN	CB-CG-OD1	7.89	137.37	121.60
1	D	329	ASN	CB-CG-ND2	-7.85	97.85	116.70
1	D	330	GLN	CG-CD-OE1	7.83	137.25	121.60
1	F	329	ASN	CA-C-O	7.82	136.53	120.10
1	D	330	GLN	CG-CD-NE2	-7.59	98.49	116.70
1	A	330	GLN	CB-CG-CD	-7.38	92.40	111.60
1	H	69	ASP	CB-CG-OD2	7.23	124.81	118.30
1	D	206	ASP	CB-CG-OD2	7.17	124.75	118.30
1	C	39	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	69	ASP	CB-CG-OD2	6.93	124.53	118.30
1	C	330	GLN	CA-CB-CG	6.92	128.63	113.40
1	H	61	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	330	GLN	CB-CA-C	-6.76	96.87	110.40
1	C	329	ASN	CB-CA-C	-6.76	96.87	110.40
1	A	117	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	329	ASN	N-CA-CB	6.61	122.50	110.60
1	C	295	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	26	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	295	ASP	CB-CG-OD2	6.45	124.10	118.30
1	C	329	ASN	CB-CG-ND2	-6.38	101.38	116.70
1	A	330	GLN	CA-CB-CG	6.35	127.38	113.40
1	G	329	ASN	CA-C-O	6.22	133.15	120.10
1	F	61	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	330	GLN	CB-CA-C	6.10	122.61	110.40
1	E	69	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	329	ASN	CB-CG-OD1	6.07	133.73	121.60
1	D	26	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	10	ASP	CB-CG-OD2	5.91	123.61	118.30
1	A	231	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	115	THR	CB-CA-C	-5.86	95.79	111.60
1	H	11	ASP	CB-CG-OD2	5.83	123.54	118.30
1	E	204	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	295	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	26	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	206	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	10	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	11	ASP	CB-CG-OD2	5.63	123.37	118.30
1	H	206	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	69	ASP	CB-CG-OD2	5.56	123.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	11	ASP	CB-CG-OD2	5.56	123.30	118.30
1	C	61	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	204	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	11	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	117	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	330	GLN	CG-CD-OE1	-5.46	110.67	121.60
1	A	11	ASP	CB-CG-OD2	5.44	123.20	118.30
1	H	204	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	117	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	91	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	222	ASP	CB-CG-OD2	5.39	123.15	118.30
1	H	295	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	10	ASP	CB-CG-OD2	5.27	123.05	118.30
1	G	117	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	329	ASN	CA-C-O	-5.24	109.10	120.10
1	D	69	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	26	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	61	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	69	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	330	GLN	CG-CD-NE2	-5.17	104.30	116.70
1	B	10	ASP	CB-CG-OD1	5.15	122.94	118.30
1	G	20	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	313	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	204	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	11	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	26	ASP	CB-CG-OD2	5.08	122.88	118.30
1	E	222	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	328	LEU	Mainchain

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	2576	0	2554	18	0
1	B	2576	0	2554	24	0
1	C	2576	0	2554	29	0
1	D	2576	0	2554	24	0
1	E	2579	0	2556	27	0
1	F	2567	0	2546	17	0
1	G	2567	0	2546	20	0
1	H	2567	0	2546	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	193	0	0	1	0
3	B	185	0	0	2	0
3	C	163	0	0	2	0
3	D	164	0	0	1	0
3	E	186	0	0	3	0
3	F	165	0	0	0	0
3	G	154	0	0	0	0
3	H	193	0	0	0	0
All	All	21995	0	20410	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (144) 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:G:297:SER:H	1:G:323:GLN:HE22	1.03	0.99
1:D:330:GLN:C	1:D:330:GLN:HE21	1.66	0.99
1:F:95:LYS:H	1:F:95:LYS:HD3	1.30	0.97
1:B:297:SER:H	1:B:323:GLN:HE22	1.10	0.94
1:E:297:SER:H	1:E:323:GLN:HE22	1.19	0.86
1:F:95:LYS:CD	1:F:95:LYS:H	1.89	0.85
1:E:303:SER:H	1:F:329:ASN:HD21	1.18	0.85
1:D:329:ASN:O	1:D:330:GLN:O	1.94	0.85
1:C:254:HIS:HD2	1:D:260:ASN:HD21	1.27	0.81
1:G:121:GLU:O	1:G:124:THR:HG22	1.82	0.80
1:G:260:ASN:HD21	1:H:254:HIS:HD2	1.29	0.79
1:E:254:HIS:HD2	1:F:260:ASN:HD21	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ARG:HH21	1:G:321:ARG:HG2	1.51	0.75
1:A:260:ASN:HD21	1:B:254:HIS:HD2	1.35	0.75
1:G:321:ARG:NH2	1:G:321:ARG:HG2	2.03	0.73
1:G:297:SER:H	1:G:323:GLN:NE2	1.85	0.73
1:D:243:LYS:HD3	1:D:247:GLU:OE1	1.89	0.72
1:C:254:HIS:CD2	1:D:260:ASN:HD21	2.09	0.71
1:F:71:VAL:HG23	1:F:77:MET:HG2	1.74	0.70
1:C:260:ASN:HD21	1:D:254:HIS:HD2	1.38	0.70
1:B:37:GLY:H	1:B:50:ASN:ND2	1.90	0.69
1:F:117:ASP:OD1	1:F:167:ARG:NH1	2.26	0.68
1:G:260:ASN:HD21	1:H:254:HIS:CD2	2.12	0.67
1:B:120:ILE:O	1:B:124:THR:HG23	1.96	0.66
1:D:50:ASN:HD22	1:D:50:ASN:H	1.41	0.65
1:D:329:ASN:O	1:D:330:GLN:C	2.35	0.65
1:H:37:GLY:H	1:H:50:ASN:ND2	1.96	0.64
1:C:260:ASN:HD21	1:D:254:HIS:CD2	2.16	0.64
1:A:1:CYS:N	3:A:525:HOH:O	2.29	0.63
1:B:264:GLY:H	1:B:273:THR:CG2	2.13	0.61
1:C:156:ILE:HD13	1:C:165:ILE:HD13	1.80	0.61
1:F:95:LYS:N	1:F:95:LYS:HD3	2.10	0.61
1:A:254:HIS:HD2	1:B:260:ASN:HD21	1.47	0.60
1:H:50:ASN:HD22	1:H:50:ASN:H	1.46	0.60
1:E:260:ASN:HD21	1:F:254:HIS:HD2	1.48	0.60
1:C:98:ARG:HD3	3:C:398:HOH:O	2.02	0.60
1:G:122:LYS:O	1:G:125:SER:HB3	2.02	0.59
1:A:254:HIS:CD2	1:B:260:ASN:HD21	2.19	0.59
1:E:294:TYR:O	1:F:254:HIS:HE1	1.85	0.59
1:C:156:ILE:HD13	1:C:165:ILE:CD1	2.32	0.59
1:E:254:HIS:CD2	1:F:260:ASN:HD21	2.16	0.59
1:A:117:ASP:OD1	1:A:167:ARG:NH1	2.36	0.59
1:C:50:ASN:HD22	1:C:50:ASN:H	1.52	0.58
1:B:297:SER:H	1:B:323:GLN:NE2	1.93	0.58
1:E:254:HIS:HE1	1:F:294:TYR:O	1.86	0.57
1:D:123:LEU:HD12	1:D:156:ILE:HD13	1.87	0.57
1:H:36:TYR:H	1:H:50:ASN:HD21	1.52	0.56
1:A:294:TYR:O	1:B:254:HIS:HE1	1.89	0.56
1:A:71:VAL:HG23	1:A:77:MET:HG2	1.88	0.55
1:C:36:TYR:H	1:C:50:ASN:HD21	1.55	0.55
1:A:117:ASP:OD1	1:A:167:ARG:CZ	2.55	0.55
1:C:254:HIS:HE1	1:D:294:TYR:O	1.88	0.54
1:C:156:ILE:CD1	1:C:165:ILE:CD1	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASN:HD21	1:B:254:HIS:CD2	2.20	0.54
1:G:117:ASP:OD2	1:G:167:ARG:NH1	2.41	0.54
1:A:117:ASP:OD1	1:A:167:ARG:NH2	2.42	0.53
1:A:181:TRP:CD1	1:D:181:TRP:CD1	2.98	0.52
1:B:308:ASN:ND2	1:B:310:ASN:H	2.07	0.52
2:E:337:CL:CL	3:E:520:HOH:O	2.56	0.52
1:C:294:TYR:O	1:D:254:HIS:HE1	1.93	0.52
1:D:50:ASN:ND2	1:D:50:ASN:H	2.07	0.52
1:G:321:ARG:HH21	1:G:321:ARG:CG	2.16	0.52
1:G:7:ARG:HD3	1:G:13:SER:OG	2.10	0.51
1:E:260:ASN:HD21	1:F:254:HIS:CD2	2.26	0.51
1:B:50:ASN:HD22	1:B:50:ASN:H	1.59	0.51
1:A:254:HIS:HE1	1:B:294:TYR:O	1.92	0.51
1:B:37:GLY:H	1:B:50:ASN:HD22	1.59	0.51
1:G:264:GLY:H	1:G:273:THR:HG23	1.76	0.51
1:D:329:ASN:C	1:D:330:GLN:O	2.49	0.51
1:E:308:ASN:ND2	1:E:310:ASN:H	2.10	0.49
1:A:156:ILE:HG12	1:A:165:ILE:CD1	2.42	0.49
1:E:50:ASN:HA	1:E:112:ASN:HD21	1.76	0.49
1:C:254:HIS:HD2	1:D:260:ASN:ND2	2.02	0.49
1:C:37:GLY:H	1:C:50:ASN:ND2	2.11	0.48
1:C:50:ASN:HA	1:C:112:ASN:HD21	1.78	0.48
1:D:36:TYR:H	1:D:50:ASN:HD21	1.61	0.48
1:E:121:GLU:HG3	3:E:447:HOH:O	2.14	0.48
1:B:95:LYS:HD2	1:B:95:LYS:N	2.29	0.48
1:E:303:SER:H	1:F:329:ASN:ND2	1.98	0.48
1:H:243:LYS:HD3	1:H:247:GLU:OE1	2.14	0.48
1:H:50:ASN:ND2	1:H:50:ASN:H	2.11	0.47
1:G:120:ILE:HG23	1:G:165:ILE:HD13	1.96	0.47
1:B:264:GLY:H	1:B:273:THR:HG23	1.79	0.47
1:D:175:ALA:HB3	1:D:225:PRO:HB3	1.95	0.47
1:G:167:ARG:HE	1:G:167:ARG:HB3	1.30	0.47
1:C:9:THR:OG1	1:C:243:LYS:HA	2.15	0.47
1:B:1:CYS:HB2	3:B:518:HOH:O	2.14	0.47
1:E:297:SER:H	1:E:323:GLN:NE2	2.00	0.47
1:E:122:LYS:O	1:E:125:SER:HB2	2.15	0.47
1:G:294:TYR:O	1:H:254:HIS:HE1	1.97	0.47
1:D:50:ASN:HA	1:D:112:ASN:HD21	1.79	0.47
1:B:1:CYS:N	3:B:518:HOH:O	2.48	0.47
1:C:154:ILE:HD12	1:C:156:ILE:HD11	1.97	0.47
1:C:50:ASN:ND2	1:C:50:ASN:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASP:OD1	1:D:167:ARG:NH1	2.48	0.46
1:E:181:TRP:CD1	1:H:181:TRP:CD1	3.04	0.46
1:D:37:GLY:H	1:D:50:ASN:ND2	2.14	0.46
1:D:1:CYS:N	3:D:501:HOH:O	2.48	0.46
1:C:329:ASN:HB2	1:C:330:GLN:H	1.57	0.46
1:C:206:ASP:HB3	3:C:465:HOH:O	2.16	0.46
1:E:224:THR:O	1:E:228:ARG:HG3	2.16	0.45
1:A:86:PHE:O	1:A:88:THR:HG22	2.17	0.45
1:F:308:ASN:ND2	1:F:310:ASN:H	2.14	0.45
1:C:175:ALA:HB3	1:C:225:PRO:HB3	1.98	0.44
1:B:36:TYR:N	1:B:50:ASN:HD21	2.16	0.44
1:A:224:THR:O	1:A:228:ARG:HG3	2.17	0.44
1:E:264:GLY:H	1:E:273:THR:HG23	1.83	0.44
1:D:241:LYS:HE2	1:D:241:LYS:CA	2.48	0.44
1:E:264:GLY:H	1:E:273:THR:CG2	2.31	0.43
1:A:50:ASN:HA	1:A:112:ASN:HD21	1.83	0.43
1:C:156:ILE:CD1	1:C:165:ILE:HD12	2.48	0.43
1:E:39:ARG:CZ	1:E:63:THR:HG21	2.48	0.43
1:C:235:TRP:CE3	1:C:235:TRP:HA	2.53	0.43
1:A:264:GLY:H	1:A:273:THR:HG23	1.84	0.43
1:E:175:ALA:HB3	1:E:225:PRO:HB3	2.01	0.43
1:H:50:ASN:HA	1:H:112:ASN:HD21	1.83	0.43
1:G:260:ASN:ND2	1:H:254:HIS:HD2	2.06	0.43
1:C:125:SER:OG	1:C:126:TYR:CE2	2.71	0.43
1:F:322:LYS:HB2	1:F:322:LYS:HE3	1.65	0.43
1:B:36:TYR:H	1:B:50:ASN:HD21	1.66	0.42
1:C:154:ILE:HG22	1:C:167:ARG:HA	2.01	0.42
1:B:122:LYS:HD3	1:B:122:LYS:HA	1.93	0.42
1:B:181:TRP:CD1	1:C:181:TRP:CD1	3.08	0.42
1:D:312:GLN:HG3	1:D:313:ASP:OD1	2.19	0.42
1:G:24:GLU:OE2	1:G:321:ARG:NH2	2.52	0.42
1:G:223:PHE:CD1	1:G:261:ILE:HG12	2.55	0.42
1:G:175:ALA:HB3	1:G:225:PRO:HB3	2.01	0.41
1:A:80:MET:HE3	1:A:106:ILE:HG12	2.01	0.41
1:C:156:ILE:CD1	1:C:165:ILE:HD13	2.48	0.41
1:C:235:TRP:HE3	1:C:235:TRP:HA	1.85	0.41
1:E:28:LYS:HB3	1:E:28:LYS:HE2	1.90	0.41
1:H:235:TRP:CE3	1:H:235:TRP:HA	2.55	0.41
1:G:122:LYS:HD3	1:G:122:LYS:HA	1.87	0.41
1:E:109:VAL:HG13	1:E:119:VAL:HG22	2.02	0.41
1:E:294:TYR:O	1:F:254:HIS:CE1	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HG23	1:C:77:MET:HG2	2.02	0.41
1:E:80:MET:C	1:E:81:LEU:HD12	2.41	0.41
1:E:160:LYS:NZ	1:E:160:LYS:CB	2.84	0.41
1:B:264:GLY:H	1:B:273:THR:HG21	1.85	0.41
1:E:94:LYS:HD2	3:E:402:HOH:O	2.21	0.41
1:F:120:ILE:O	1:F:124:THR:HG23	2.21	0.40
1:E:219:LEU:HD21	1:E:231:ARG:HG2	2.04	0.40
1:H:176:SER:HB3	1:H:177:PRO:HA	2.03	0.40
1:B:50:ASN:HA	1:B:112:ASN:HD21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/335 (98%)	316 (96%)	12 (4%)	0	100	100
1	B	328/335 (98%)	318 (97%)	10 (3%)	0	100	100
1	C	328/335 (98%)	317 (97%)	11 (3%)	0	100	100
1	D	328/335 (98%)	318 (97%)	10 (3%)	0	100	100
1	E	329/335 (98%)	317 (96%)	12 (4%)	0	100	100
1	F	327/335 (98%)	317 (97%)	10 (3%)	0	100	100
1	G	327/335 (98%)	317 (97%)	10 (3%)	0	100	100
1	H	327/335 (98%)	315 (96%)	12 (4%)	0	100	100
All	All	2622/2680 (98%)	2535 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	286/291 (98%)	275 (96%)	11 (4%)	40	17
1	B	286/291 (98%)	277 (97%)	9 (3%)	47	25
1	C	286/291 (98%)	276 (96%)	10 (4%)	43	20
1	D	286/291 (98%)	272 (95%)	14 (5%)	31	11
1	E	287/291 (99%)	277 (96%)	10 (4%)	43	20
1	F	285/291 (98%)	271 (95%)	14 (5%)	31	11
1	G	285/291 (98%)	272 (95%)	13 (5%)	33	12
1	H	285/291 (98%)	275 (96%)	10 (4%)	43	20
All	All	2286/2328 (98%)	2195 (96%)	91 (4%)	39	16

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	23	MET
1	A	82	TYR
1	A	88	THR
1	A	95	LYS
1	A	134	ILE
1	A	143	HIS
1	A	235	TRP
1	A	309	LEU
1	A	313	ASP
1	A	330	GLN
1	B	17	ARG
1	B	43	LYS
1	B	45	ASN
1	B	50	ASN
1	B	82	TYR
1	B	95	LYS
1	B	122	LYS
1	B	143	HIS

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Mol	Chain	Res	Type
1	B	167	ARG
1	C	17	ARG
1	C	50	ASN
1	C	82	TYR
1	C	95	LYS
1	C	98	ARG
1	C	123	LEU
1	C	130	ASN
1	C	134	ILE
1	C	143	HIS
1	C	243	LYS
1	D	17	ARG
1	D	23	MET
1	D	28	LYS
1	D	50	ASN
1	D	82	TYR
1	D	92	GLU
1	D	143	HIS
1	D	201	MET
1	D	235	TRP
1	D	241	LYS
1	D	243	LYS
1	D	273	THR
1	D	312	GLN
1	D	330	GLN
1	E	17	ARG
1	E	23	MET
1	E	45[A]	ASN
1	E	45[B]	ASN
1	E	69	ASP
1	E	82	TYR
1	E	123	LEU
1	E	143	HIS
1	E	160	LYS
1	E	235	TRP
1	F	17	ARG
1	F	23	MET
1	F	24	GLU
1	F	28	LYS
1	F	82	TYR
1	F	95	LYS
1	F	135	ILE

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Mol	Chain	Res	Type
1	F	143	HIS
1	F	160	LYS
1	F	235	TRP
1	F	241	LYS
1	F	308	ASN
1	F	322	LYS
1	F	329	ASN
1	G	7	ARG
1	G	17	ARG
1	G	24	GLU
1	G	44	GLU
1	G	82	TYR
1	G	95	LYS
1	G	122	LYS
1	G	143	HIS
1	G	163	ILE
1	G	167	ARG
1	G	235	TRP
1	G	282	MET
1	G	321	ARG
1	H	11	ASP
1	H	17	ARG
1	H	23	MET
1	H	50	ASN
1	H	82	TYR
1	H	88	THR
1	H	95	LYS
1	H	143	HIS
1	H	243	LYS
1	H	321	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	A	198	GLN
1	A	254	HIS
1	A	330	GLN
1	B	49	ASN
1	B	50	ASN
1	B	112	ASN
1	B	130	ASN

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Mol	Chain	Res	Type
1	B	254	HIS
1	B	308	ASN
1	B	323	GLN
1	C	49	ASN
1	C	50	ASN
1	C	112	ASN
1	C	185	ASN
1	C	254	HIS
1	C	330	GLN
1	D	50	ASN
1	D	112	ASN
1	D	130	ASN
1	D	185	ASN
1	D	198	GLN
1	D	212	GLN
1	D	251	ASN
1	D	254	HIS
1	D	327	GLN
1	D	330	GLN
1	E	112	ASN
1	E	166	HIS
1	E	183	GLN
1	E	185	ASN
1	E	254	HIS
1	E	308	ASN
1	E	323	GLN
1	E	327	GLN
1	F	185	ASN
1	F	251	ASN
1	F	254	HIS
1	F	308	ASN
1	F	329	ASN
1	G	49	ASN
1	G	112	ASN
1	G	130	ASN
1	G	212	GLN
1	G	251	ASN
1	G	323	GLN
1	H	35	ASN
1	H	45	ASN
1	H	49	ASN
1	H	50	ASN

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Mol	Chain	Res	Type
1	H	112	ASN
1	H	185	ASN
1	H	198	GLN
1	H	254	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	330/335 (98%)	-0.21	3 (0%)	85	88	9, 17, 32, 37	0
1	B	330/335 (98%)	-0.16	3 (0%)	85	88	10, 16, 29, 36	0
1	C	330/335 (98%)	0.11	5 (1%)	76	80	10, 18, 31, 39	0
1	D	330/335 (98%)	-0.06	5 (1%)	76	80	10, 18, 32, 42	0
1	E	330/335 (98%)	-0.13	4 (1%)	81	85	10, 17, 30, 43	0
1	F	329/335 (98%)	-0.03	3 (0%)	85	88	11, 17, 31, 40	0
1	G	329/335 (98%)	-0.12	3 (0%)	85	88	12, 18, 34, 41	0
1	H	329/335 (98%)	-0.30	1 (0%)	94	95	10, 17, 31, 40	0
All	All	2637/2680 (98%)	-0.11	27 (1%)	84	87	9, 17, 32, 43	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	330	GLN	6.1
1	D	330	GLN	5.6
1	A	330	GLN	4.7
1	E	330	GLN	4.4
1	B	330	GLN	4.0
1	C	123	LEU	3.7
1	E	95	LYS	3.4
1	F	96	GLY	2.9
1	G	95	LYS	2.9
1	F	95	LYS	2.8
1	A	95	LYS	2.8
1	F	135	ILE	2.7
1	E	123	LEU	2.7
1	D	312	GLN	2.6
1	H	95	LYS	2.5
1	E	312	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	134	ILE	2.5
1	C	95	LYS	2.5
1	C	312	GLN	2.4
1	G	161	THR	2.3
1	B	167	ARG	2.3
1	D	95	LYS	2.2
1	B	95	LYS	2.2
1	D	329	ASN	2.1
1	D	161	THR	2.1
1	G	124	THR	2.0
1	A	161	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	A	336	1/1	0.97	0.07	-0.64	23,23,23,23	0
2	CL	G	336	1/1	0.94	0.07	-0.98	24,24,24,24	0
2	CL	E	337	1/1	0.96	0.07	-1.53	23,23,23,23	0
2	CL	B	336	1/1	0.98	0.07	-1.77	24,24,24,24	0
2	CL	H	336	1/1	0.96	0.06	-1.98	25,25,25,25	0
2	CL	C	336	1/1	0.98	0.06	-3.91	24,24,24,24	0
2	CL	C	337	1/1	0.98	0.06	-4.20	23,23,23,23	0
2	CL	E	336	1/1	0.99	0.04	-4.41	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.