Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 12:44 PM EDT

PDB ID	:	2O1W
Title	:	Structure of N-terminal plus middle domains (N+M) of GRP94
Authors	:	Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on	:	2006-11-29
Resolution	:	3.40 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 (1)) were used in the production of this report:

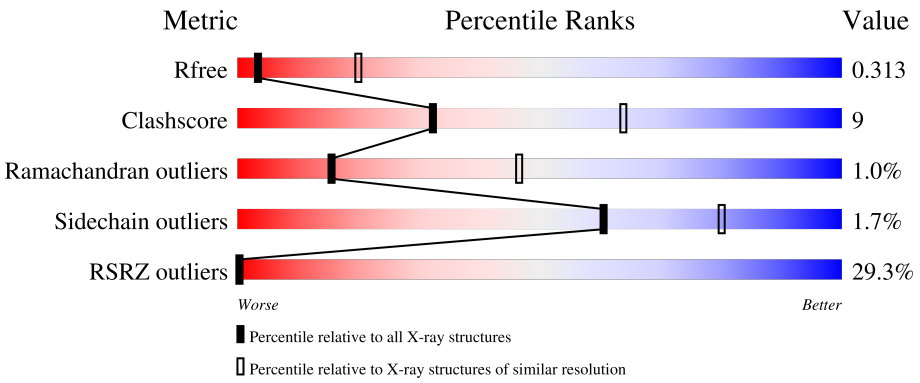
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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% 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	506	22% 66% 15% • 18%
1	B	506	17% 68% 23% • 7%
1	C	506	20% 65% 17% 18%
1	D	506	26% 67% 15% 18%
1	E	506	38% 69% 14% 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17042 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3333	2133	552	638	10	0	1	0
1	B	469	3710	2373	615	709	13	0	0	0
1	C	416	3333	2133	552	638	10	0	0	0
1	D	416	3333	2133	552	638	10	0	0	0
1	E	416	3333	2133	552	638	10	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	expression tag	UNP P41148
A	53	GLY	-	expression tag	UNP P41148
A	54	SER	-	expression tag	UNP P41148
A	55	SER	-	expression tag	UNP P41148
A	56	HIS	-	expression tag	UNP P41148
A	57	HIS	-	expression tag	UNP P41148
A	58	HIS	-	expression tag	UNP P41148
A	59	HIS	-	expression tag	UNP P41148
A	60	HIS	-	expression tag	UNP P41148
A	61	HIS	-	expression tag	UNP P41148
A	62	SER	-	expression tag	UNP P41148
A	63	SER	-	expression tag	UNP P41148
A	64	GLY	-	expression tag	UNP P41148
A	65	LEU	-	expression tag	UNP P41148
A	66	VAL	-	expression tag	UNP P41148
A	67	PRO	-	expression tag	UNP P41148
A	68	ARG	-	expression tag	UNP P41148
A	69	GLY	-	expression tag	UNP P41148
A	70	SER	-	expression tag	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	HIS	-	expression tag	UNP P41148
A	72	MET	-	expression tag	UNP P41148
A	287	GLY	-	see remark 999	UNP P41148
A	288	GLY	-	see remark 999	UNP P41148
A	289	GLY	-	see remark 999	UNP P41148
A	290	GLY	-	see remark 999	UNP P41148
B	52	MET	-	expression tag	UNP P41148
B	53	GLY	-	expression tag	UNP P41148
B	54	SER	-	expression tag	UNP P41148
B	55	SER	-	expression tag	UNP P41148
B	56	HIS	-	expression tag	UNP P41148
B	57	HIS	-	expression tag	UNP P41148
B	58	HIS	-	expression tag	UNP P41148
B	59	HIS	-	expression tag	UNP P41148
B	60	HIS	-	expression tag	UNP P41148
B	61	HIS	-	expression tag	UNP P41148
B	62	SER	-	expression tag	UNP P41148
B	63	SER	-	expression tag	UNP P41148
B	64	GLY	-	expression tag	UNP P41148
B	65	LEU	-	expression tag	UNP P41148
B	66	VAL	-	expression tag	UNP P41148
B	67	PRO	-	expression tag	UNP P41148
B	68	ARG	-	expression tag	UNP P41148
B	69	GLY	-	expression tag	UNP P41148
B	70	SER	-	expression tag	UNP P41148
B	71	HIS	-	expression tag	UNP P41148
B	72	MET	-	expression tag	UNP P41148
B	287	GLY	-	see remark 999	UNP P41148
B	288	GLY	-	see remark 999	UNP P41148
B	289	GLY	-	see remark 999	UNP P41148
B	290	GLY	-	see remark 999	UNP P41148
C	52	MET	-	expression tag	UNP P41148
C	53	GLY	-	expression tag	UNP P41148
C	54	SER	-	expression tag	UNP P41148
C	55	SER	-	expression tag	UNP P41148
C	56	HIS	-	expression tag	UNP P41148
C	57	HIS	-	expression tag	UNP P41148
C	58	HIS	-	expression tag	UNP P41148
C	59	HIS	-	expression tag	UNP P41148
C	60	HIS	-	expression tag	UNP P41148
C	61	HIS	-	expression tag	UNP P41148
C	62	SER	-	expression tag	UNP P41148

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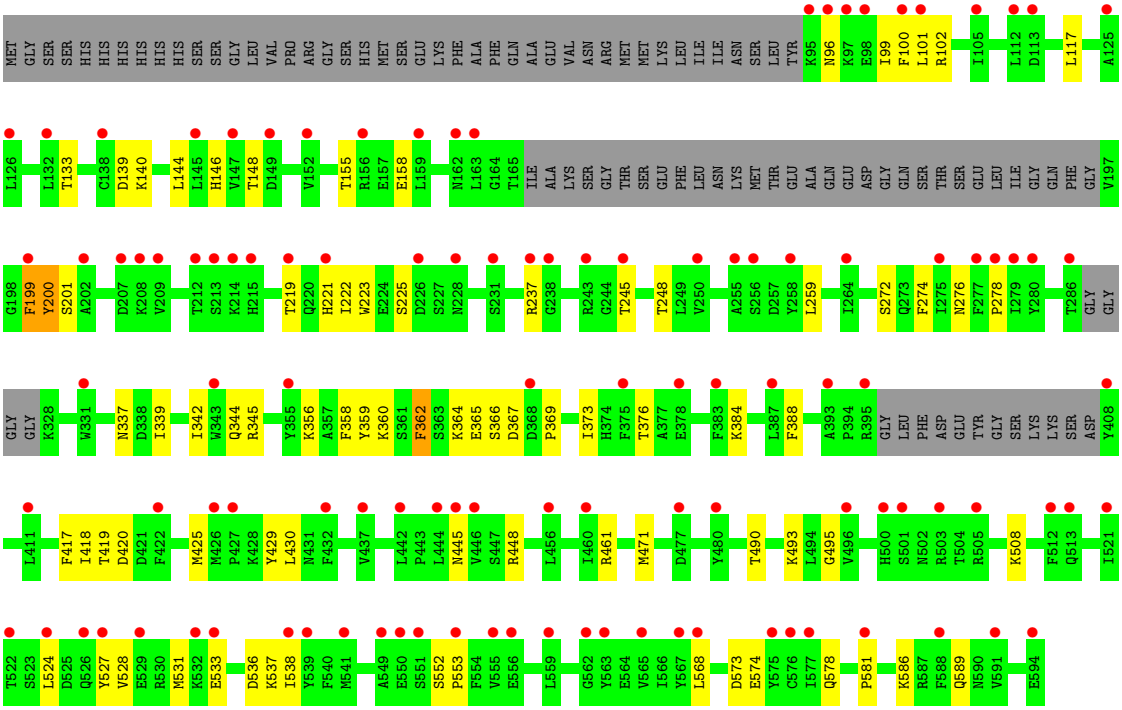
Chain	Residue	Modelled	Actual	Comment	Reference
C	63	SER	-	expression tag	UNP P41148
C	64	GLY	-	expression tag	UNP P41148
C	65	LEU	-	expression tag	UNP P41148
C	66	VAL	-	expression tag	UNP P41148
C	67	PRO	-	expression tag	UNP P41148
C	68	ARG	-	expression tag	UNP P41148
C	69	GLY	-	expression tag	UNP P41148
C	70	SER	-	expression tag	UNP P41148
C	71	HIS	-	expression tag	UNP P41148
C	72	MET	-	expression tag	UNP P41148
C	287	GLY	-	see remark 999	UNP P41148
C	288	GLY	-	see remark 999	UNP P41148
C	289	GLY	-	see remark 999	UNP P41148
C	290	GLY	-	see remark 999	UNP P41148
D	52	MET	-	expression tag	UNP P41148
D	53	GLY	-	expression tag	UNP P41148
D	54	SER	-	expression tag	UNP P41148
D	55	SER	-	expression tag	UNP P41148
D	56	HIS	-	expression tag	UNP P41148
D	57	HIS	-	expression tag	UNP P41148
D	58	HIS	-	expression tag	UNP P41148
D	59	HIS	-	expression tag	UNP P41148
D	60	HIS	-	expression tag	UNP P41148
D	61	HIS	-	expression tag	UNP P41148
D	62	SER	-	expression tag	UNP P41148
D	63	SER	-	expression tag	UNP P41148
D	64	GLY	-	expression tag	UNP P41148
D	65	LEU	-	expression tag	UNP P41148
D	66	VAL	-	expression tag	UNP P41148
D	67	PRO	-	expression tag	UNP P41148
D	68	ARG	-	expression tag	UNP P41148
D	69	GLY	-	expression tag	UNP P41148
D	70	SER	-	expression tag	UNP P41148
D	71	HIS	-	expression tag	UNP P41148
D	72	MET	-	expression tag	UNP P41148
D	287	GLY	-	see remark 999	UNP P41148
D	288	GLY	-	see remark 999	UNP P41148
D	289	GLY	-	see remark 999	UNP P41148
D	290	GLY	-	see remark 999	UNP P41148

3 Residue-property plots (i)

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

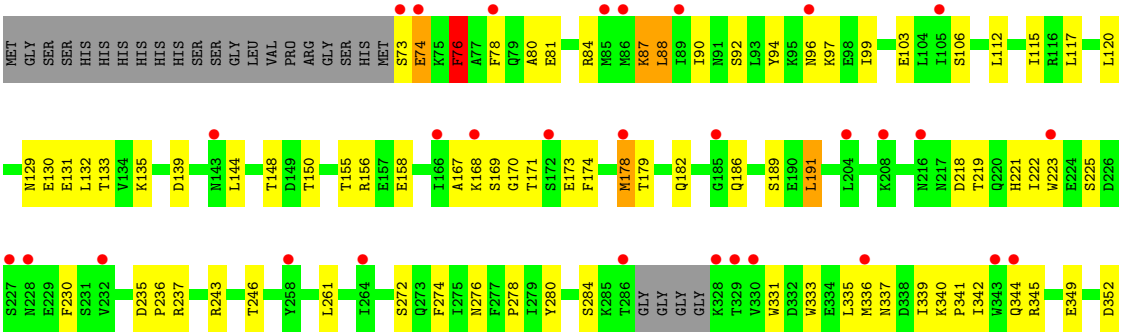
• Molecule 1: Endoplasmin

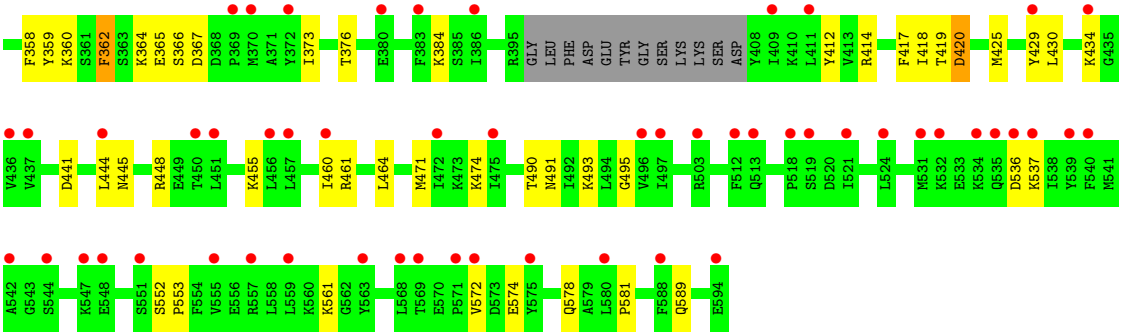
Chain A:



• Molecule 1: Endoplasmin

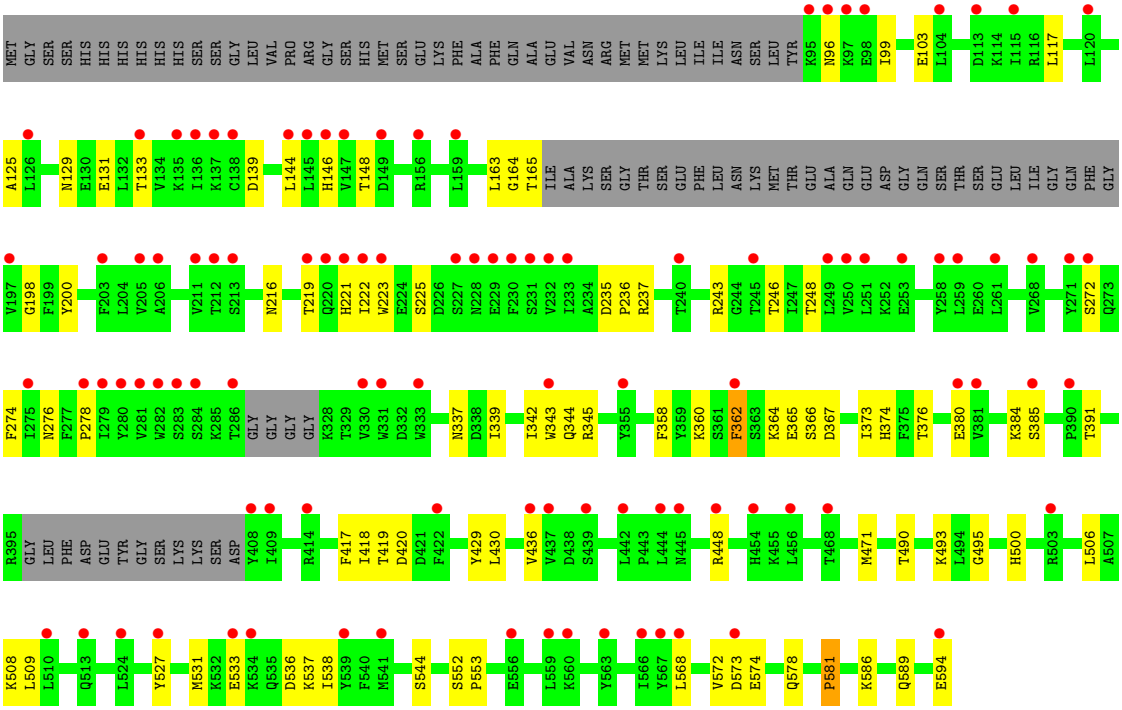
Chain B:





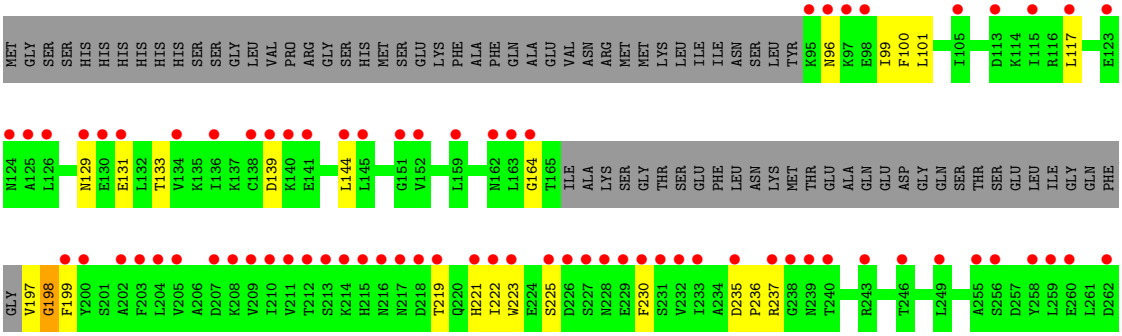
- Molecule 1: Endoplasmin

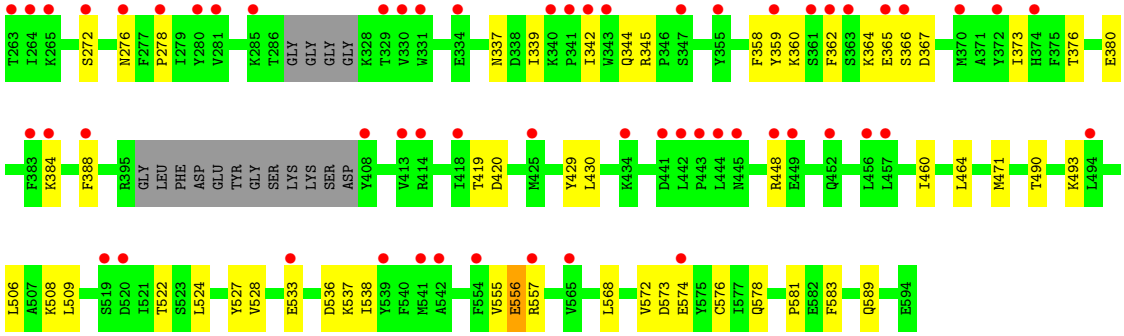
Chain C:



- Molecule 1: Endoplasmin

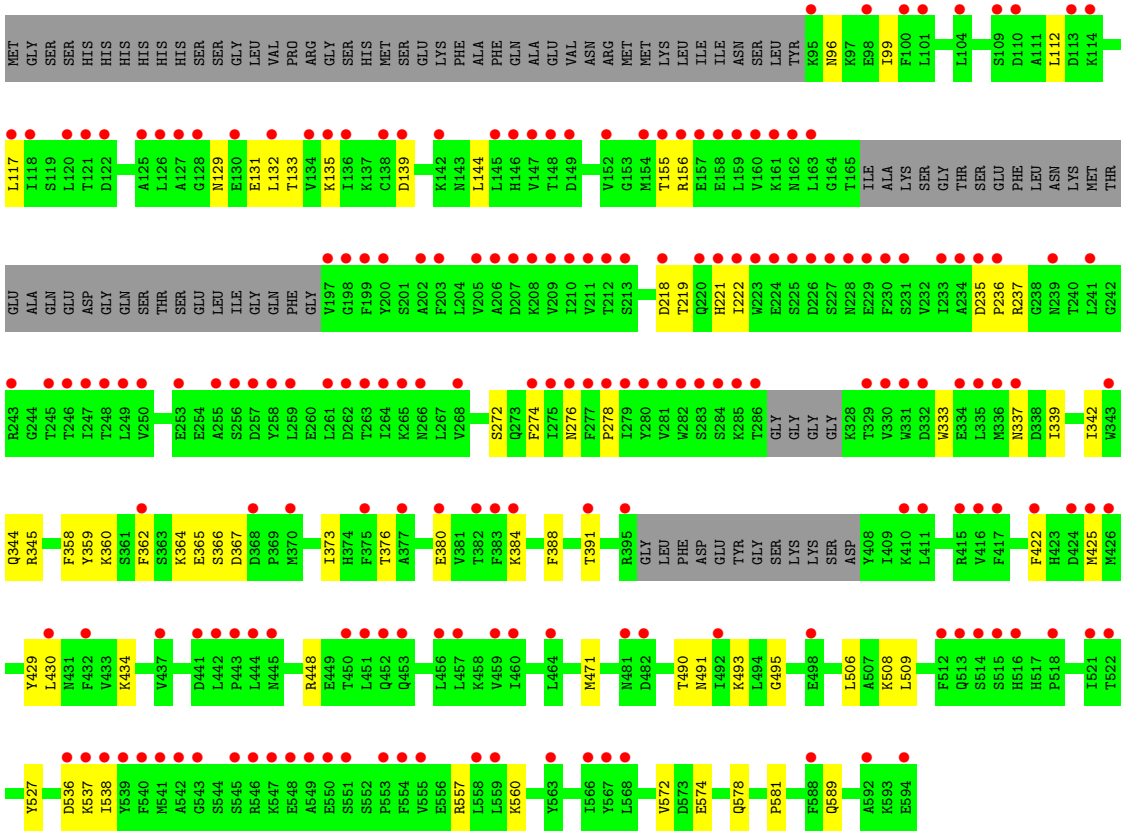
Chain D:





- Molecule 1: Endoplasmin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	210.33Å 137.50Å 133.15Å 90.00° 124.10° 90.00°	Depositor
Resolution (Å)	47.30 – 3.40 47.73 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.30-3.40) 98.1 (47.73-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.314 , 0.332 0.294 , 0.313	Depositor DCC
R_{free} test set	2122 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	148.6	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 247.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17042	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.49	0/3400	0.56	0/4599
1	B	0.83	9/3783 (0.2%)	0.71	3/5117 (0.1%)
1	C	0.57	3/3400 (0.1%)	0.56	0/4599
1	D	0.53	1/3400 (0.0%)	0.58	1/4599 (0.0%)
1	E	0.37	0/3400	0.52	0/4599
All	All	0.58	13/17383 (0.1%)	0.59	4/23513 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	LYS	CE-NZ	18.68	1.95	1.49
1	C	164	GLY	C-N	12.88	1.63	1.34
1	B	87	LYS	CD-CE	10.94	1.78	1.51
1	B	87	LYS	CG-CD	10.16	1.86	1.52
1	C	165	THR	CB-OG1	8.56	1.60	1.43
1	C	165	THR	C-O	7.99	1.38	1.23
1	B	81	GLU	CD-OE1	7.93	1.34	1.25
1	B	76	PHE	CE2-CZ	6.58	1.49	1.37
1	D	576	CYS	CB-SG	-6.52	1.71	1.82
1	B	81	GLU	CD-OE2	6.52	1.32	1.25
1	B	74	GLU	CG-CD	5.94	1.60	1.51
1	B	76	PHE	CG-CD2	5.87	1.47	1.38
1	B	76	PHE	CG-CD1	5.26	1.46	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	87	LYS	CD-CE-NZ	-10.41	87.76	111.70
1	B	76	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	B	87	LYS	CG-CD-CE	-5.73	94.70	111.90
1	D	557	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	3333	0	3257	52	1
1	B	3710	0	3611	111	5
1	C	3333	0	3258	82	1
1	D	3333	0	3258	48	0
1	E	3333	0	3258	47	3
All	All	17042	0	16642	297	5

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 9.

All (297) 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:B:87:LYS:CE	1:B:87:LYS:CD	1.78	1.61
1:B:87:LYS:CD	1:B:87:LYS:CG	1.87	1.49
1:B:455:LYS:CB	1:C:594:GLU:HB2	1.45	1.44
1:B:414:ARG:NH2	1:C:578:GLN:HG2	1.38	1.36
1:B:414:ARG:NH2	1:C:578:GLN:CG	1.89	1.34
1:B:87:LYS:CE	1:B:87:LYS:NZ	1.95	1.28
1:D:366:SER:O	1:E:366:SER:O	1.56	1.18
1:B:414:ARG:HH21	1:C:578:GLN:CB	1.64	1.10
1:B:445:ASN:HB3	1:C:581:PRO:CB	1.82	1.09
1:B:445:ASN:HB3	1:C:581:PRO:HB3	1.24	1.09
1:B:445:ASN:CB	1:C:581:PRO:HG3	1.81	1.09
1:B:445:ASN:CB	1:C:581:PRO:HB3	1.84	1.06
1:B:445:ASN:CB	1:C:581:PRO:CB	2.34	1.05
1:B:278:PRO:HD3	1:B:339:ILE:HD12	1.45	0.99
1:B:414:ARG:HH21	1:C:578:GLN:HB3	1.22	0.99
1:B:414:ARG:HH21	1:C:578:GLN:CG	1.62	0.99
1:B:455:LYS:CB	1:C:594:GLU:CB	2.42	0.98
1:B:445:ASN:CB	1:C:581:PRO:CG	2.41	0.97
1:B:445:ASN:HB3	1:C:581:PRO:CG	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:GLU:OE1	1:D:533:GLU:HB2	1.67	0.94
1:B:414:ARG:HH22	1:C:578:GLN:HG2	0.85	0.93
1:E:278:PRO:HD3	1:E:339:ILE:HD12	1.50	0.91
1:B:445:ASN:CG	1:C:581:PRO:HG3	1.89	0.90
1:B:445:ASN:HB3	1:C:581:PRO:HG3	1.54	0.89
1:B:222:ILE:HD11	1:B:237:ARG:HH21	1.36	0.88
1:D:278:PRO:HD3	1:D:339:ILE:HD12	1.56	0.88
1:A:278:PRO:HD3	1:A:339:ILE:HD12	1.53	0.88
1:C:278:PRO:HD3	1:C:339:ILE:HD12	1.54	0.87
1:B:445:ASN:HB2	1:C:581:PRO:CB	2.04	0.86
1:B:364:LYS:C	1:B:366:SER:H	1.79	0.85
1:B:414:ARG:HH22	1:C:578:GLN:CG	1.65	0.84
1:A:533:GLU:HB2	1:E:380:GLU:OE1	1.78	0.83
1:B:445:ASN:HB2	1:C:581:PRO:CA	2.07	0.83
1:C:364:LYS:C	1:C:366:SER:H	1.82	0.83
1:E:364:LYS:C	1:E:366:SER:H	1.81	0.82
1:B:222:ILE:HD11	1:B:237:ARG:NH2	1.94	0.81
1:B:441:ASP:HA	1:C:578:GLN:HE22	1.46	0.79
1:B:78:PHE:HZ	1:B:225:SER:HG	1.31	0.79
1:A:364:LYS:C	1:A:366:SER:H	1.83	0.79
1:B:414:ARG:NH2	1:C:578:GLN:CD	2.34	0.78
1:D:364:LYS:C	1:D:366:SER:H	1.85	0.78
1:A:222:ILE:HD11	1:A:237:ARG:HH21	1.49	0.78
1:B:344:GLN:OE1	1:B:384:LYS:HD2	1.87	0.74
1:D:222:ILE:HD11	1:D:237:ARG:HH21	1.53	0.74
1:E:222:ILE:HD11	1:E:237:ARG:HH21	1.52	0.74
1:C:222:ILE:HD11	1:C:237:ARG:HH21	1.54	0.72
1:B:441:ASP:HA	1:C:578:GLN:NE2	2.04	0.72
1:B:414:ARG:NH2	1:C:578:GLN:HB3	2.02	0.71
1:B:414:ARG:NH2	1:C:578:GLN:CB	2.35	0.71
1:E:272:SER:HB3	1:E:337:ASN:HB3	1.72	0.71
1:B:87:LYS:CE	1:B:87:LYS:CG	2.68	0.71
1:B:99:ILE:HD12	1:B:189:SER:HB2	1.72	0.71
1:A:272:SER:HB3	1:A:337:ASN:HB3	1.73	0.70
1:B:272:SER:HB3	1:B:337:ASN:HB3	1.74	0.69
1:C:272:SER:HB3	1:C:337:ASN:HB3	1.73	0.69
1:B:364:LYS:O	1:B:366:SER:N	2.22	0.69
1:A:508:LYS:NZ	1:E:508:LYS:NZ	2.42	0.68
1:B:87:LYS:CD	1:B:87:LYS:CB	2.72	0.67
1:A:508:LYS:NZ	1:E:508:LYS:HZ3	1.92	0.67
1:D:272:SER:HB3	1:D:337:ASN:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLU:HB3	1:C:198:GLY:O	1.94	0.66
1:E:364:LYS:O	1:E:366:SER:N	2.25	0.66
1:B:167:ALA:O	1:B:169:SER:N	2.27	0.66
1:B:87:LYS:CD	1:B:87:LYS:NZ	2.59	0.66
1:C:373:ILE:HB	1:C:471:MET:HB2	1.79	0.65
1:A:508:LYS:HZ1	1:E:508:LYS:HZ3	1.44	0.65
1:E:342:ILE:HA	1:E:345:ARG:HD3	1.78	0.64
1:B:76:PHE:CD1	1:B:76:PHE:N	2.64	0.64
1:A:342:ILE:HA	1:A:345:ARG:HD3	1.79	0.64
1:D:344:GLN:OE1	1:D:384:LYS:HD2	1.98	0.64
1:C:537:LYS:HE2	1:C:589:GLN:HB2	1.78	0.63
1:A:364:LYS:O	1:A:366:SER:N	2.30	0.63
1:A:508:LYS:HZ1	1:E:508:LYS:NZ	1.97	0.63
1:D:373:ILE:HB	1:D:471:MET:HB2	1.81	0.62
1:D:527:TYR:CE2	1:D:538:ILE:HG23	2.35	0.62
1:B:373:ILE:HB	1:B:471:MET:HB2	1.81	0.62
1:A:222:ILE:HD11	1:A:237:ARG:NH2	2.15	0.62
1:B:445:ASN:O	1:C:581:PRO:HB3	1.99	0.62
1:E:364:LYS:C	1:E:366:SER:N	2.53	0.62
1:A:537:LYS:HE2	1:A:589:GLN:HB2	1.82	0.62
1:B:276:ASN:O	1:B:339:ILE:HG13	1.99	0.62
1:C:342:ILE:HA	1:C:345:ARG:HD3	1.81	0.61
1:B:364:LYS:C	1:B:366:SER:N	2.52	0.61
1:B:445:ASN:HB2	1:C:581:PRO:CG	2.27	0.61
1:E:537:LYS:HE2	1:E:589:GLN:HB2	1.82	0.61
1:B:342:ILE:HA	1:B:345:ARG:HD3	1.82	0.61
1:B:537:LYS:HE2	1:B:589:GLN:HB2	1.83	0.61
1:D:574:GLU:O	1:D:578:GLN:HB2	2.01	0.61
1:E:373:ILE:HB	1:E:471:MET:HB2	1.83	0.61
1:B:96:ASN:O	1:B:99:ILE:HG22	2.00	0.60
1:D:342:ILE:HA	1:D:345:ARG:HD3	1.84	0.60
1:B:88:LEU:HB3	1:B:178:MET:HE3	1.84	0.60
1:B:445:ASN:HB2	1:C:581:PRO:HA	1.82	0.60
1:A:360:LYS:HG2	1:A:366:SER:HA	1.83	0.60
1:C:364:LYS:C	1:C:366:SER:N	2.54	0.60
1:A:364:LYS:C	1:A:366:SER:N	2.55	0.60
1:A:425:MET:O	1:A:461:ARG:HD2	2.01	0.59
1:D:537:LYS:HE2	1:D:589:GLN:HB2	1.84	0.59
1:E:222:ILE:HD11	1:E:237:ARG:NH2	2.16	0.59
1:C:222:ILE:HD11	1:C:237:ARG:NH2	2.17	0.59
1:A:429:TYR:CE1	1:A:430:LEU:HG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:HB	1:A:471:MET:HB2	1.84	0.59
1:D:222:ILE:HD11	1:D:237:ARG:NH2	2.18	0.59
1:D:364:LYS:O	1:D:366:SER:N	2.32	0.59
1:E:574:GLU:O	1:E:578:GLN:HB2	2.03	0.58
1:A:574:GLU:O	1:A:578:GLN:HB2	2.03	0.58
1:C:364:LYS:O	1:C:366:SER:N	2.29	0.58
1:C:574:GLU:O	1:C:578:GLN:HB2	2.04	0.58
1:A:276:ASN:O	1:A:339:ILE:HG13	2.04	0.57
1:B:360:LYS:HG2	1:B:366:SER:HA	1.85	0.57
1:D:364:LYS:C	1:D:366:SER:N	2.57	0.57
1:B:78:PHE:HZ	1:B:225:SER:OG	1.86	0.57
1:B:76:PHE:HB2	1:B:230:PHE:CZ	2.40	0.57
1:B:574:GLU:O	1:B:578:GLN:HB2	2.05	0.57
1:C:360:LYS:HG2	1:C:366:SER:HA	1.87	0.56
1:D:197:VAL:HG23	1:D:198:GLY:H	1.70	0.56
1:B:445:ASN:ND2	1:C:581:PRO:HG3	2.20	0.56
1:A:199:PHE:CD2	1:A:200:TYR:N	2.74	0.56
1:B:429:TYR:CE1	1:B:430:LEU:HG	2.41	0.56
1:E:276:ASN:O	1:E:339:ILE:HG13	2.07	0.55
1:C:429:TYR:CE1	1:C:430:LEU:HG	2.42	0.55
1:B:92:SER:HB3	1:B:182:GLN:NE2	2.22	0.54
1:E:155:THR:HG22	1:E:218:ASP:HB2	1.89	0.54
1:B:274:PHE:CE1	1:B:358:PHE:HB2	2.42	0.54
1:D:429:TYR:CE1	1:D:430:LEU:HG	2.42	0.54
1:E:344:GLN:OE1	1:E:384:LYS:HD2	2.09	0.53
1:E:429:TYR:CE1	1:E:430:LEU:HG	2.44	0.52
1:B:135:LYS:HB3	1:B:333:TRP:CH2	2.45	0.52
1:A:96:ASN:O	1:A:99:ILE:HG22	2.09	0.51
1:D:524:LEU:O	1:D:528:VAL:HG23	2.11	0.51
1:B:112:LEU:HD22	1:B:132:LEU:HB3	1.93	0.51
1:B:80:ALA:O	1:B:84:ARG:NH1	2.43	0.51
1:C:362:PHE:HD2	1:C:362:PHE:O	1.94	0.51
1:E:360:LYS:HG2	1:E:366:SER:HA	1.91	0.51
1:A:418:ILE:HG22	1:A:419:THR:HG22	1.93	0.51
1:B:139:ASP:HB3	1:B:144:LEU:HB2	1.92	0.50
1:B:129:ASN:OD1	1:B:131:GLU:HG2	2.12	0.50
1:B:219:THR:O	1:B:221:HIS:ND1	2.42	0.50
1:A:199:PHE:O	1:A:201:SER:N	2.45	0.50
1:B:429:TYR:CD2	1:B:495:GLY:HA2	2.46	0.50
1:D:133:THR:HG22	1:D:278:PRO:HG2	1.93	0.50
1:D:360:LYS:HG2	1:D:366:SER:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:221:HIS:ND1	2.45	0.50
1:C:536:ASP:OD2	1:C:537:LYS:HG2	2.12	0.49
1:C:358:PHE:CE1	1:C:362:PHE:HE1	2.31	0.49
1:D:568:LEU:HD22	1:D:573:ASP:HB3	1.94	0.49
1:D:276:ASN:O	1:D:339:ILE:HG13	2.12	0.49
1:B:536:ASP:OD2	1:B:537:LYS:HG2	2.13	0.49
1:B:76:PHE:N	1:B:76:PHE:HD1	2.10	0.48
1:B:148:THR:HG23	1:B:246:THR:OG1	2.12	0.48
1:A:344:GLN:OE1	1:A:384:LYS:HD2	2.13	0.48
1:B:133:THR:HG22	1:B:278:PRO:HG2	1.95	0.48
1:B:155:THR:OG1	1:B:158:GLU:HG3	2.13	0.48
1:E:96:ASN:O	1:E:99:ILE:HG22	2.13	0.48
1:C:96:ASN:O	1:C:99:ILE:HG22	2.13	0.48
1:D:96:ASN:O	1:D:99:ILE:HG22	2.13	0.48
1:E:536:ASP:OD2	1:E:537:LYS:HG2	2.14	0.48
1:B:429:TYR:O	1:B:491:ASN:HB3	2.14	0.48
1:C:276:ASN:O	1:C:339:ILE:HG13	2.14	0.48
1:D:536:ASP:OD2	1:D:537:LYS:HG2	2.13	0.48
1:C:133:THR:HG22	1:C:278:PRO:HG2	1.96	0.47
1:C:274:PHE:CE1	1:C:358:PHE:HB2	2.49	0.47
1:B:417:PHE:O	1:B:418:ILE:HD13	2.14	0.47
1:B:490:THR:HA	1:B:493:LYS:HE3	1.96	0.47
1:C:344:GLN:OE1	1:C:384:LYS:HD2	2.13	0.47
1:C:367:ASP:OD1	1:C:367:ASP:N	2.47	0.47
1:B:223:TRP:NE1	1:B:230:PHE:CD1	2.83	0.47
1:A:417:PHE:O	1:A:418:ILE:HD13	2.15	0.47
1:A:536:ASP:OD2	1:A:537:LYS:HG2	2.15	0.47
1:B:76:PHE:HB2	1:B:230:PHE:CE2	2.50	0.47
1:C:223:TRP:CH2	1:C:225:SER:HB3	2.50	0.47
1:D:129:ASN:OD1	1:D:131:GLU:HG2	2.15	0.47
1:B:150:THR:O	1:B:243:ARG:NH2	2.45	0.47
1:C:506:LEU:HA	1:C:509:LEU:HD12	1.97	0.47
1:A:140:LYS:HA	1:A:259:LEU:HD22	1.97	0.46
1:A:155:THR:OG1	1:A:158:GLU:HG3	2.16	0.46
1:D:358:PHE:CE1	1:D:362:PHE:HE1	2.33	0.46
1:B:135:LYS:HD3	1:B:333:TRP:CZ2	2.51	0.46
1:C:235:ASP:HA	1:C:236:PRO:HD2	1.84	0.46
1:C:508:LYS:HZ1	1:D:508:LYS:HZ1	1.62	0.46
1:C:219:THR:O	1:C:221:HIS:ND1	2.48	0.46
1:D:555:VAL:O	1:D:556:GLU:C	2.53	0.46
1:A:133:THR:HG22	1:A:278:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD12	1:B:336:MET:H	1.80	0.46
1:D:524:LEU:HB3	1:D:583:PHE:CE2	2.51	0.46
1:B:155:THR:HG22	1:B:218:ASP:HB2	1.97	0.46
1:E:362:PHE:HD2	1:E:362:PHE:O	1.99	0.46
1:C:429:TYR:CD2	1:C:495:GLY:HA2	2.51	0.46
1:B:460:ILE:O	1:B:464:LEU:HG	2.17	0.45
1:E:490:THR:HA	1:E:493:LYS:HE3	1.97	0.45
1:E:133:THR:HG22	1:E:278:PRO:HG2	1.98	0.45
1:A:99:ILE:HD11	1:A:102:ARG:NH2	2.31	0.45
1:C:129:ASN:OD1	1:C:131:GLU:HG2	2.17	0.45
1:C:380:GLU:OE1	1:D:533:GLU:CB	2.51	0.45
1:C:533:GLU:HB2	1:D:380:GLU:OE1	2.16	0.45
1:C:163:LEU:HA	1:C:200:TYR:OH	2.16	0.45
1:B:167:ALA:C	1:B:169:SER:H	2.17	0.45
1:C:417:PHE:O	1:C:418:ILE:HD13	2.16	0.45
1:A:359:TYR:HB2	1:A:388:PHE:CE1	2.52	0.45
1:A:490:THR:HA	1:A:493:LYS:HE3	1.98	0.45
1:B:359:TYR:HE1	1:B:434:LYS:HD2	1.82	0.45
1:B:425:MET:O	1:B:461:ARG:HD2	2.16	0.45
1:B:235:ASP:HA	1:B:236:PRO:HD2	1.81	0.45
1:A:367:ASP:OD1	1:A:367:ASP:N	2.47	0.44
1:D:533:GLU:HA	1:D:533:GLU:OE2	2.17	0.44
1:D:367:ASP:OD1	1:D:367:ASP:N	2.50	0.44
1:E:235:ASP:HA	1:E:236:PRO:HD2	1.85	0.44
1:E:358:PHE:CE1	1:E:362:PHE:HE1	2.36	0.44
1:A:199:PHE:HD2	1:A:200:TYR:N	2.15	0.44
1:A:362:PHE:HD2	1:A:362:PHE:O	2.01	0.44
1:B:218:ASP:OD1	1:B:219:THR:N	2.48	0.44
1:D:359:TYR:HB2	1:D:388:PHE:CE1	2.53	0.44
1:E:367:ASP:OD1	1:E:367:ASP:N	2.51	0.44
1:A:146:HIS:CE1	1:A:248:THR:HG23	2.53	0.44
1:D:490:THR:HG23	1:D:572:VAL:HG11	2.00	0.44
1:C:343:TRP:CD2	1:C:436:VAL:HG21	2.53	0.43
1:B:243:ARG:CZ	1:B:243:ARG:HB3	2.49	0.43
1:C:362:PHE:O	1:C:362:PHE:CD2	2.71	0.43
1:D:366:SER:HB3	1:E:366:SER:HB3	2.01	0.43
1:B:156:ARG:HG3	1:B:221:HIS:CD2	2.54	0.43
1:B:278:PRO:HB2	1:B:280:TYR:CE2	2.53	0.43
1:C:148:THR:HG23	1:C:246:THR:OG1	2.19	0.43
1:D:506:LEU:O	1:D:509:LEU:N	2.38	0.43
1:D:506:LEU:HA	1:D:509:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:THR:O	1:E:221:HIS:ND1	2.52	0.43
1:C:490:THR:HA	1:C:493:LYS:HE3	2.01	0.43
1:D:219:THR:O	1:D:221:HIS:ND1	2.52	0.43
1:B:419:THR:OG1	1:B:420:ASP:N	2.52	0.43
1:D:235:ASP:HA	1:D:236:PRO:HD2	1.84	0.43
1:A:527:TYR:CE2	1:A:538:ILE:HG23	2.54	0.43
1:A:139:ASP:HB3	1:A:144:LEU:HB2	2.01	0.42
1:B:367:ASP:N	1:B:367:ASP:OD1	2.51	0.42
1:A:358:PHE:CE1	1:A:362:PHE:HE1	2.38	0.42
1:B:552:SER:HA	1:B:553:PRO:HD3	1.93	0.42
1:B:120:LEU:HD22	1:B:444:LEU:HD11	2.01	0.42
1:D:490:THR:HA	1:D:493:LYS:HE3	2.01	0.42
1:D:419:THR:OG1	1:D:420:ASP:N	2.52	0.42
1:B:130:GLU:OE1	1:C:500:HIS:NE2	2.52	0.42
1:C:568:LEU:HD22	1:C:573:ASP:HB3	2.00	0.42
1:D:164:GLY:HA2	1:D:230:PHE:CE2	2.54	0.42
1:C:527:TYR:CE2	1:C:538:ILE:HG23	2.54	0.42
1:C:531:MET:HE1	1:C:586:LYS:HD2	2.01	0.42
1:D:100:PHE:CG	1:D:101:LEU:N	2.88	0.42
1:A:552:SER:HA	1:A:553:PRO:HD3	1.92	0.42
1:B:235:ASP:OD2	1:B:237:ARG:NH2	2.52	0.42
1:B:362:PHE:HD2	1:B:362:PHE:O	2.02	0.42
1:E:135:LYS:HB3	1:E:333:TRP:CH2	2.55	0.42
1:B:131:GLU:CG	1:B:150:THR:HG21	2.50	0.42
1:E:490:THR:HG23	1:E:572:VAL:HG11	2.01	0.42
1:A:429:TYR:CD2	1:A:495:GLY:HA2	2.55	0.41
1:E:156:ARG:HB2	1:E:221:HIS:NE2	2.35	0.41
1:C:129:ASN:O	1:C:243:ARG:NH1	2.39	0.41
1:C:374:HIS:HD2	1:C:385:SER:O	2.03	0.41
1:C:552:SER:HA	1:C:553:PRO:HD3	1.89	0.41
1:D:460:ILE:O	1:D:464:LEU:HG	2.21	0.41
1:C:139:ASP:HB3	1:C:144:LEU:HB2	2.02	0.41
1:E:429:TYR:O	1:E:491:ASN:HB3	2.20	0.41
1:E:429:TYR:CD2	1:E:495:GLY:HA2	2.55	0.41
1:A:100:PHE:CG	1:A:101:LEU:N	2.88	0.41
1:B:94:TYR:HB2	1:B:97:LYS:HZ1	1.85	0.41
1:E:156:ARG:HB2	1:E:221:HIS:CE1	2.55	0.41
1:A:274:PHE:CE1	1:A:358:PHE:HB2	2.55	0.41
1:B:174:PHE:HE2	1:B:191:LEU:O	2.03	0.41
1:B:261:LEU:HD11	1:B:331:TRP:CZ3	2.55	0.41
1:E:274:PHE:CE1	1:E:358:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LYS:HG2	1:A:369:PRO:HD2	2.03	0.41
1:A:531:MET:HE1	1:A:586:LYS:HD2	2.02	0.41
1:B:171:THR:HG22	1:B:171:THR:O	2.21	0.41
1:B:340:LYS:HA	1:B:341:PRO:HD3	1.95	0.41
1:C:125:ALA:O	1:C:216:ASN:ND2	2.51	0.41
1:E:129:ASN:OD1	1:E:131:GLU:HG2	2.20	0.41
1:B:112:LEU:O	1:B:115:ILE:HG22	2.21	0.41
1:B:490:THR:HG23	1:B:572:VAL:HG11	2.02	0.41
1:E:112:LEU:HD22	1:E:132:LEU:HB3	2.02	0.41
1:E:359:TYR:HB2	1:E:388:PHE:CE1	2.55	0.41
1:B:103:GLU:O	1:B:106:SER:HB3	2.21	0.41
1:B:135:LYS:HD3	1:B:333:TRP:CE2	2.55	0.41
1:C:419:THR:OG1	1:C:420:ASP:N	2.54	0.41
1:D:223:TRP:CH2	1:D:225:SER:HB3	2.55	0.41
1:A:148:THR:HA	1:A:245:THR:O	2.21	0.40
1:A:568:LEU:HD22	1:A:573:ASP:HB3	2.02	0.40
1:B:130:GLU:OE1	1:C:500:HIS:CE1	2.74	0.40
1:D:362:PHE:HD2	1:D:362:PHE:O	2.03	0.40
1:E:139:ASP:HB3	1:E:144:LEU:HB2	2.03	0.40
1:E:359:TYR:HE1	1:E:434:LYS:HD2	1.86	0.40
1:E:527:TYR:CE2	1:E:538:ILE:HG23	2.57	0.40
1:B:429:TYR:CD1	1:B:430:LEU:HG	2.57	0.40
1:B:445:ASN:O	1:C:581:PRO:CB	2.67	0.40
1:A:524:LEU:O	1:A:528:VAL:HG23	2.21	0.40
1:C:490:THR:HG23	1:C:572:VAL:HG11	2.02	0.40
1:D:139:ASP:HB3	1:D:144:LEU:HB2	2.03	0.40
1:A:223:TRP:CH2	1:A:225:SER:HB3	2.55	0.40
1:B:156:ARG:HB2	1:B:221:HIS:CE1	2.56	0.40
1:C:146:HIS:CE1	1:C:248:THR:HG23	2.57	0.40
1:E:422:PHE:HB3	1:E:425:MET:HG2	2.04	0.40
1:E:506:LEU:HA	1:E:509:LEU:HD12	2.03	0.40
1:A:419:THR:OG1	1:A:420:ASP:N	2.54	0.40

All (5) 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:349:GLU:O	1:E:560:LYS:NZ[4_555]	1.61	0.59
1:B:561:LYS:NZ	1:C:544:SER:OG[2_655]	2.04	0.16
1:A:445:ASN:OD1	1:B:284:SER:OG[4_545]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:GLU:C	1:E:560:LYS:NZ[4_555]	2.12	0.08
1:B:352:ASP:N	1:E:557:ARG:NH2[4_555]	2.13	0.07

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	408/506 (81%)	381 (93%)	23 (6%)	4 (1%)	15	46
1	B	463/506 (92%)	409 (88%)	47 (10%)	7 (2%)	10	36
1	C	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	29	61
1	D	408/506 (81%)	379 (93%)	24 (6%)	5 (1%)	13	41
1	E	408/506 (81%)	379 (93%)	27 (7%)	2 (0%)	29	61
All	All	2095/2530 (83%)	1927 (92%)	148 (7%)	20 (1%)	15	46

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PHE
1	B	168	LYS
1	B	365	GLU
1	A	200	TYR
1	A	365	GLU
1	B	186	GLN
1	C	365	GLU
1	D	198	GLY
1	E	365	GLU
1	A	581	PRO
1	C	581	PRO
1	D	199	PHE
1	D	365	GLU
1	B	581	PRO

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Mol	Chain	Res	Type
1	D	581	PRO
1	E	581	PRO
1	B	173	GLU
1	B	474	LYS
1	D	556	GLU
1	B	170	GLY

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	365/456 (80%)	361 (99%)	4 (1%)	73	86
1	B	400/456 (88%)	386 (96%)	14 (4%)	36	65
1	C	365/456 (80%)	360 (99%)	5 (1%)	67	83
1	D	365/456 (80%)	361 (99%)	4 (1%)	73	86
1	E	365/456 (80%)	361 (99%)	4 (1%)	73	86
All	All	1860/2280 (82%)	1829 (98%)	31 (2%)	60	80

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	362	PHE
1	A	376	THR
1	A	448	ARG
1	B	73	SER
1	B	74	GLU
1	B	76	PHE
1	B	88	LEU
1	B	90	ILE
1	B	117	LEU
1	B	178	MET
1	B	179	THR
1	B	191	LEU

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Mol	Chain	Res	Type
1	B	362	PHE
1	B	376	THR
1	B	412	TYR
1	B	420	ASP
1	B	448	ARG
1	C	117	LEU
1	C	362	PHE
1	C	376	THR
1	C	391	THR
1	C	448	ARG
1	D	117	LEU
1	D	376	THR
1	D	448	ARG
1	D	522	THR
1	E	117	LEU
1	E	376	THR
1	E	391	THR
1	E	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	C	578	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	164:GLY	C	165:THR	N	1.63

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	416/506 (82%)	1.40	112 (26%)	0	0	179, 194, 209, 226	0
1	B	469/506 (92%)	1.22	84 (17%)	1	1	179, 195, 223, 253	0
1	C	416/506 (82%)	1.21	103 (24%)	0	0	179, 194, 209, 226	0
1	D	416/506 (82%)	1.65	132 (31%)	0	0	179, 194, 209, 226	0
1	E	416/506 (82%)	2.99	194 (46%)	0	0	179, 194, 209, 226	0
All	All	2133/2530 (84%)	1.68	625 (29%)	0	0	179, 194, 211, 253	0

All (625) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	285	LYS	54.7
1	E	286	THR	26.6
1	E	198	GLY	21.1
1	E	247	ILE	16.7
1	E	281	VAL	16.4
1	E	277	PHE	16.1
1	E	147	VAL	14.1
1	D	138	CYS	13.9
1	E	163	LEU	13.7
1	D	163	LEU	13.6
1	E	280	TYR	13.4
1	E	264	ILE	13.2
1	E	284	SER	13.2
1	E	205	VAL	12.7
1	E	226	ASP	11.6
1	D	258	TYR	11.2
1	E	234	ALA	11.0
1	D	259	LEU	11.0
1	E	334	GLU	10.4
1	E	228	ASN	10.4

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Mol	Chain	Res	Type	RSRZ
1	E	227	SER	10.3
1	E	279	ILE	10.0
1	C	253	GLU	10.0
1	B	73	SER	9.6
1	E	258	TYR	9.6
1	E	383	PHE	9.4
1	B	380	GLU	9.4
1	E	335	LEU	9.3
1	E	206	ALA	9.3
1	D	152	VAL	9.3
1	E	452	GLN	9.2
1	A	594	GLU	9.1
1	E	443	PRO	9.1
1	E	235	ASP	9.1
1	E	246	THR	9.1
1	E	442	LEU	8.9
1	E	266	ASN	8.8
1	E	199	PHE	8.7
1	E	212	THR	8.7
1	E	202	ALA	8.6
1	E	262	ASP	8.5
1	E	542	ALA	8.5
1	E	233	ILE	8.4
1	D	442	LEU	8.4
1	E	125	ALA	8.3
1	A	159	LEU	8.2
1	C	281	VAL	8.1
1	D	222	ILE	8.1
1	E	245	THR	8.1
1	A	125	ALA	8.0
1	E	136	ILE	7.9
1	B	329	THR	7.7
1	E	451	LEU	7.7
1	E	330	VAL	7.5
1	B	548	GLU	7.4
1	E	126	LEU	7.4
1	D	330	VAL	7.3
1	E	208	LYS	7.2
1	E	100	PHE	7.1
1	E	248	THR	7.1
1	B	563	TYR	7.0
1	E	197	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	225	SER	7.0
1	C	444	LEU	7.0
1	A	521	ILE	6.9
1	C	230	PHE	6.8
1	E	263	THR	6.8
1	E	154	MET	6.8
1	E	278	PRO	6.8
1	E	265	LYS	6.7
1	B	286	THR	6.6
1	E	249	LEU	6.6
1	E	152	VAL	6.6
1	D	205	VAL	6.5
1	E	329	THR	6.5
1	A	163	LEU	6.5
1	D	131	GLU	6.5
1	D	225	SER	6.4
1	B	519	SER	6.3
1	E	207	ASP	6.3
1	D	208	LYS	6.2
1	D	230	PHE	6.2
1	E	382	THR	6.2
1	A	126	LEU	6.2
1	E	155	THR	6.1
1	E	541	MET	6.1
1	C	136	ILE	6.1
1	E	113	ASP	6.1
1	A	97	LYS	6.1
1	E	162	ASN	6.0
1	A	562	GLY	6.0
1	E	588	PHE	6.0
1	E	160	VAL	6.0
1	D	223	TRP	6.0
1	E	200	TYR	5.9
1	E	239	ASN	5.9
1	C	203	PHE	5.9
1	E	550	GLU	5.9
1	C	227	SER	5.8
1	A	208	LYS	5.8
1	E	268	VAL	5.8
1	D	444	LEU	5.8
1	A	95	LYS	5.7
1	D	232	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	134	VAL	5.7
1	C	228	ASN	5.7
1	A	496	VAL	5.6
1	D	237	ARG	5.6
1	A	162	ASN	5.6
1	E	422	PHE	5.6
1	A	237	ARG	5.5
1	D	211	VAL	5.5
1	E	236	PRO	5.5
1	A	533	GLU	5.5
1	E	213	SER	5.5
1	E	558	LEU	5.4
1	E	149	ASP	5.4
1	D	162	ASN	5.4
1	D	159	LEU	5.4
1	E	498	GLU	5.4
1	C	146	HIS	5.4
1	E	481	ASN	5.4
1	A	541	MET	5.3
1	E	110	ASP	5.3
1	A	549	ALA	5.3
1	D	278	PRO	5.3
1	C	138	CYS	5.3
1	C	144	LEU	5.3
1	E	276	ASN	5.1
1	E	549	ALA	5.1
1	D	331	TRP	5.1
1	B	178	MET	5.1
1	A	551	SER	5.0
1	D	212	THR	5.0
1	D	445	ASN	5.0
1	D	141	GLU	5.0
1	E	209	VAL	5.0
1	D	115	ILE	4.9
1	B	551	SER	4.9
1	C	448	ARG	4.9
1	E	548	GLU	4.9
1	B	451	LEU	4.8
1	E	211	VAL	4.8
1	D	285	LYS	4.8
1	A	277	PHE	4.8
1	D	227	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	283	SER	4.8
1	D	260	GLU	4.8
1	E	566	ILE	4.8
1	D	202	ALA	4.7
1	D	151	GLY	4.7
1	D	209	VAL	4.7
1	E	553	PRO	4.7
1	E	568	LEU	4.6
1	E	231	SER	4.6
1	E	456	LEU	4.6
1	D	255	ALA	4.6
1	C	390	PRO	4.6
1	E	377	ALA	4.5
1	D	98	GLU	4.5
1	B	571	PRO	4.5
1	D	221	HIS	4.5
1	E	563	TYR	4.5
1	D	213	SER	4.5
1	E	203	PHE	4.5
1	D	443	PRO	4.5
1	E	229	GLU	4.5
1	C	409	ILE	4.5
1	C	137	LYS	4.5
1	D	203	PHE	4.5
1	C	221	HIS	4.4
1	E	444	LEU	4.4
1	A	96	ASN	4.4
1	E	567	TYR	4.4
1	A	213	SER	4.4
1	D	280	TYR	4.4
1	E	138	CYS	4.4
1	C	222	ILE	4.4
1	C	282	TRP	4.4
1	E	145	LEU	4.3
1	D	228	ASN	4.3
1	A	445	ASN	4.3
1	A	343	TRP	4.3
1	D	124	ASN	4.3
1	C	145	LEU	4.3
1	D	125	ALA	4.3
1	C	219	THR	4.3
1	A	563	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	207	ASP	4.2
1	A	539	TYR	4.2
1	D	262	ASP	4.2
1	E	250	VAL	4.2
1	A	279	ILE	4.2
1	C	422	PHE	4.2
1	D	219	THR	4.2
1	E	157	GLU	4.2
1	E	464	LEU	4.1
1	A	147	VAL	4.1
1	E	460	ILE	4.1
1	B	328	LYS	4.1
1	D	215	HIS	4.1
1	E	512	PHE	4.1
1	A	132	LEU	4.1
1	D	276	ASN	4.0
1	E	594	GLU	4.0
1	B	575	TYR	4.0
1	D	519	SER	4.0
1	A	228	ASN	4.0
1	C	454	HIS	4.0
1	B	429	TYR	4.0
1	E	104	LEU	4.0
1	E	259	LEU	4.0
1	C	213	SER	4.0
1	E	274	PHE	3.9
1	C	534	LYS	3.9
1	C	533	GLU	3.9
1	E	224	GLU	3.9
1	E	450	THR	3.9
1	A	553	PRO	3.9
1	E	411	LEU	3.9
1	A	432	PHE	3.8
1	A	286	THR	3.8
1	E	156	ARG	3.8
1	C	568	LEU	3.8
1	B	535	GLN	3.8
1	C	220	GLN	3.8
1	D	448	ARG	3.8
1	E	257	ASP	3.8
1	C	333	TRP	3.8
1	C	231	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	101	LEU	3.8
1	E	521	ILE	3.8
1	B	568	LEU	3.7
1	B	227	SER	3.7
1	E	426	MET	3.7
1	E	95	LYS	3.7
1	B	588	PHE	3.7
1	C	331	TRP	3.7
1	E	336	MET	3.7
1	D	117	LEU	3.7
1	E	117	LEU	3.7
1	B	228	ASN	3.7
1	D	126	LEU	3.7
1	B	74	GLU	3.6
1	A	567	TYR	3.6
1	B	503	ARG	3.6
1	E	559	LEU	3.6
1	D	199	PHE	3.6
1	A	214	LYS	3.6
1	D	414	ARG	3.6
1	C	259	LEU	3.6
1	E	343	TRP	3.6
1	E	253	GLU	3.5
1	A	559	LEU	3.5
1	A	231	SER	3.5
1	B	456	LEU	3.5
1	E	146	HIS	3.5
1	A	145	LEU	3.5
1	D	218	ASP	3.5
1	B	559	LEU	3.5
1	D	226	ASP	3.5
1	D	554	PHE	3.5
1	A	226	ASP	3.4
1	E	445	ASN	3.4
1	D	341	PRO	3.4
1	B	569	THR	3.4
1	E	223	TRP	3.4
1	A	529	GLU	3.4
1	B	204	LEU	3.4
1	D	233	ILE	3.4
1	D	140	LYS	3.4
1	D	343	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	164	GLY	3.4
1	E	139	ASP	3.3
1	E	539	TYR	3.3
1	D	240	THR	3.3
1	D	97	LYS	3.3
1	B	86	MET	3.3
1	C	343	TRP	3.3
1	A	446	VAL	3.3
1	E	555	VAL	3.3
1	E	545	SER	3.3
1	A	138	CYS	3.3
1	B	540	PHE	3.3
1	D	264	ILE	3.3
1	B	531	MET	3.3
1	C	147	VAL	3.3
1	A	383	PHE	3.3
1	B	78	PHE	3.3
1	B	330	VAL	3.3
1	E	222	ILE	3.3
1	E	380	GLU	3.3
1	D	229	GLU	3.3
1	B	232	VAL	3.3
1	A	256	SER	3.2
1	D	238	GLY	3.2
1	A	442	LEU	3.2
1	B	532	LYS	3.2
1	E	120	LEU	3.2
1	E	159	LEU	3.2
1	B	539	TYR	3.2
1	C	240	THR	3.2
1	D	129	ASN	3.2
1	C	385	SER	3.2
1	C	223	TRP	3.2
1	D	383	PHE	3.2
1	B	594	GLU	3.2
1	E	142	LYS	3.2
1	C	206	ALA	3.2
1	E	221	HIS	3.2
1	A	331	TRP	3.2
1	E	282	TRP	3.2
1	A	98	GLU	3.2
1	C	442	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	556	GLU	3.2
1	A	156	ARG	3.1
1	C	279	ILE	3.1
1	E	375	PHE	3.1
1	C	439	SER	3.1
1	B	518	PRO	3.1
1	D	541	MET	3.1
1	C	284	SER	3.1
1	E	538	ILE	3.1
1	D	413	VAL	3.1
1	C	445	ASN	3.1
1	E	241	LEU	3.1
1	E	543	GLY	3.1
1	B	444	LEU	3.1
1	C	524	LEU	3.1
1	B	185	GLY	3.1
1	E	118	ILE	3.1
1	D	359	TYR	3.1
1	A	245	THR	3.1
1	C	513	GLN	3.1
1	D	539	TYR	3.0
1	D	214	LYS	3.0
1	E	98	GLU	3.0
1	C	250	VAL	3.0
1	B	172	SER	3.0
1	C	272	SER	3.0
1	D	239	ASN	3.0
1	A	255	ALA	3.0
1	A	581	PRO	3.0
1	D	136	ILE	3.0
1	A	513	GLN	3.0
1	B	537	LYS	3.0
1	D	130	GLU	3.0
1	D	340	LYS	3.0
1	E	243	ARG	3.0
1	A	395	ARG	3.0
1	A	568	LEU	3.0
1	A	243	ARG	3.0
1	E	459	VAL	3.0
1	D	457	LEU	3.0
1	D	334	GLU	3.0
1	C	232	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	426	MET	3.0
1	E	391	THR	3.0
1	C	258	TYR	2.9
1	B	89	ILE	2.9
1	C	355	TYR	2.9
1	B	166	ILE	2.9
1	C	135	LYS	2.9
1	E	592	ALA	2.9
1	C	280	TYR	2.9
1	A	378	GLU	2.9
1	E	230	PHE	2.9
1	C	268	VAL	2.9
1	E	410	LYS	2.9
1	A	460	ILE	2.8
1	D	355	TYR	2.8
1	C	97	LYS	2.8
1	A	100	PHE	2.8
1	A	512	PHE	2.8
1	C	362	PHE	2.8
1	D	434	LYS	2.8
1	C	566	ILE	2.8
1	E	210	ILE	2.8
1	A	524	LEU	2.8
1	E	148	THR	2.8
1	A	565	VAL	2.8
1	D	263	THR	2.8
1	A	258	TYR	2.8
1	A	501	SER	2.8
1	B	370	MET	2.8
1	C	560	LYS	2.8
1	B	557	ARG	2.8
1	C	414	ARG	2.8
1	E	522	THR	2.8
1	D	134	VAL	2.8
1	E	536	ASP	2.8
1	A	215	HIS	2.8
1	E	425	MET	2.7
1	C	283	SER	2.7
1	D	243	ARG	2.7
1	D	329	THR	2.7
1	C	159	LEU	2.7
1	E	537	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	563	TYR	2.7
1	A	105	ILE	2.7
1	E	121	THR	2.7
1	E	158	GLU	2.7
1	C	559	LEU	2.7
1	A	555	VAL	2.7
1	C	539	TYR	2.7
1	A	149	ASP	2.7
1	D	456	LEU	2.7
1	C	567	TYR	2.7
1	E	370	MET	2.7
1	D	96	ASN	2.7
1	A	538	ILE	2.7
1	C	278	PRO	2.7
1	B	475	ILE	2.7
1	E	122	ASP	2.6
1	C	381	VAL	2.6
1	A	355	TYR	2.6
1	B	457	LEU	2.6
1	A	207	ASP	2.6
1	D	139	ASP	2.6
1	B	344	GLN	2.6
1	A	393	ALA	2.6
1	A	437	VAL	2.6
1	B	572	VAL	2.6
1	B	524	LEU	2.6
1	A	591	VAL	2.6
1	C	286	THR	2.6
1	C	205	VAL	2.6
1	C	275	ILE	2.6
1	D	113	ASP	2.6
1	C	271	TYR	2.6
1	D	216	ASN	2.6
1	A	101	LEU	2.6
1	A	480	TYR	2.6
1	A	576	CYS	2.6
1	E	457	LEU	2.6
1	B	544	SER	2.6
1	A	503	ARG	2.6
1	C	126	LEU	2.6
1	A	444	LEU	2.5
1	A	280	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	2.5
1	D	281	VAL	2.5
1	C	408	TYR	2.5
1	B	512	PHE	2.5
1	D	370	MET	2.5
1	B	411	LEU	2.5
1	C	233	ILE	2.5
1	A	278	PRO	2.5
1	D	256	SER	2.5
1	E	256	SER	2.5
1	E	482	ASP	2.5
1	D	249	LEU	2.5
1	D	217	ASN	2.5
1	D	363	SER	2.5
1	B	343	TRP	2.5
1	E	492	ILE	2.5
1	C	541	MET	2.5
1	D	565	VAL	2.5
1	E	432	PHE	2.5
1	A	522	THR	2.5
1	C	115	ILE	2.5
1	A	202	ALA	2.5
1	A	387	LEU	2.5
1	E	127	ALA	2.5
1	B	536	ASP	2.5
1	D	365	GLU	2.5
1	A	408	TYR	2.4
1	D	542	ALA	2.4
1	A	264	ILE	2.4
1	B	460	ILE	2.4
1	C	330	VAL	2.4
1	B	168	LYS	2.4
1	D	265	LYS	2.4
1	E	514	SER	2.4
1	D	557	ARG	2.4
1	A	588	PHE	2.4
1	D	95	LYS	2.4
1	D	425	MET	2.4
1	E	114	LYS	2.4
1	A	527	TYR	2.4
1	B	521	ILE	2.4
1	A	112	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	331	TRP	2.4
1	D	449	GLU	2.4
1	E	547	LYS	2.4
1	A	411	LEU	2.4
1	E	368	ASP	2.3
1	D	533	GLU	2.3
1	E	554	PHE	2.3
1	D	272	SER	2.3
1	E	518	PRO	2.3
1	E	384	LYS	2.3
1	C	573	ASP	2.3
1	D	520	ASP	2.3
1	E	220	GLN	2.3
1	E	332	ASP	2.3
1	C	229	GLU	2.3
1	E	546	ARG	2.3
1	C	510	LEU	2.3
1	D	388	PHE	2.3
1	A	575	TYR	2.3
1	E	453	GLN	2.3
1	B	497	ILE	2.3
1	C	261	LEU	2.3
1	A	212	THR	2.3
1	B	437	VAL	2.3
1	A	427	PRO	2.3
1	D	231	SER	2.3
1	E	551	SER	2.3
1	E	441	ASP	2.3
1	D	494	LEU	2.3
1	B	436	VAL	2.3
1	C	594	GLU	2.3
1	A	456	LEU	2.3
1	D	408	TYR	2.3
1	D	452	GLN	2.3
1	C	212	THR	2.2
1	A	577	ILE	2.2
1	C	436	VAL	2.2
1	E	255	ALA	2.2
1	A	368	ASP	2.2
1	C	437	VAL	2.2
1	E	128	GLY	2.2
1	E	109	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	145	LEU	2.2
1	B	223	TRP	2.2
1	A	199	PHE	2.2
1	C	96	ASN	2.2
1	C	95	LYS	2.2
1	C	249	LEU	2.2
1	E	261	LEU	2.2
1	B	383	PHE	2.2
1	B	372	TYR	2.2
1	C	149	ASP	2.2
1	B	450	THR	2.2
1	C	456	LEU	2.2
1	A	221	HIS	2.2
1	B	496	VAL	2.2
1	D	574	GLU	2.2
1	E	430	LEU	2.2
1	E	513	GLN	2.2
1	B	534	LYS	2.2
1	C	197	VAL	2.2
1	E	437	VAL	2.2
1	B	542	ALA	2.2
1	C	133	THR	2.2
1	B	85	MET	2.2
1	B	386	ILE	2.2
1	D	144	LEU	2.2
1	A	532	LYS	2.2
1	E	218	ASP	2.2
1	B	143	ASN	2.2
1	A	250	VAL	2.2
1	C	556	GLU	2.2
1	E	130	GLU	2.2
1	E	415	ARG	2.2
1	E	362	PHE	2.2
1	D	123	GLU	2.2
1	E	395	ARG	2.2
1	A	477	ASP	2.2
1	A	550	GLU	2.2
1	D	235	ASP	2.2
1	E	417	PHE	2.1
1	D	200	TYR	2.1
1	A	209	VAL	2.1
1	A	238	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	113	ASP	2.1
1	A	375	PHE	2.1
1	C	245	THR	2.1
1	C	503	ARG	2.1
1	C	527	TYR	2.1
1	D	384	LYS	2.1
1	A	275	ILE	2.1
1	B	513	GLN	2.1
1	B	547	LYS	2.1
1	E	135	LYS	2.1
1	E	161	LYS	2.1
1	E	515	SER	2.1
1	D	362	PHE	2.1
1	D	372	TYR	2.1
1	B	409	ILE	2.1
1	E	337	ASN	2.1
1	C	104	LEU	2.1
1	E	416	VAL	2.1
1	A	526	GLN	2.1
1	B	336	MET	2.1
1	D	361	SER	2.1
1	D	105	ILE	2.1
1	D	210	ILE	2.1
1	E	424	ASP	2.1
1	E	132	LEU	2.1
1	A	505	ARG	2.1
1	D	204	LEU	2.1
1	E	516	HIS	2.1
1	B	208	LYS	2.1
1	D	347	SER	2.1
1	E	275	ILE	2.1
1	B	96	ASN	2.1
1	B	434	LYS	2.1
1	A	152	VAL	2.1
1	B	369	PRO	2.1
1	C	120	LEU	2.1
1	B	258	TYR	2.0
1	D	246	THR	2.0
1	E	540	PHE	2.0
1	D	374	HIS	2.0
1	B	105	ILE	2.0
1	B	216	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	500	HIS	2.0
1	C	98	GLU	2.0
1	D	441	ASP	2.0
1	B	555	VAL	2.0
1	C	211	VAL	2.0
1	B	264	ILE	2.0
1	B	472	ILE	2.0
1	B	580	LEU	2.0
1	D	418	ILE	2.0
1	A	422	PHE	2.0
1	A	219	THR	2.0
1	C	468	THR	2.0
1	C	156	ARG	2.0
1	D	366	SER	2.0
1	D	342	ILE	2.0
1	C	380	GLU	2.0
1	C	251	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.