



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 05:40 PM EDT

PDB ID : 3VR5
Title : Crystal structure of nucleotide-free *Enterococcus hirae* V1-ATPase [eV1(L)]
Authors : Saijo, S.; Arai, S.; Suzuki, K.; Mizutani, K.; Kakinuma, Y.; Ishizuka-Katsura, Y.; Ohsawa, N.; Terada, T.; Shirouzu, M.; Yokoyama, S.; Iwata, S.; Yamato, I.; Murata, T.
Deposited on : 2012-04-03
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-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

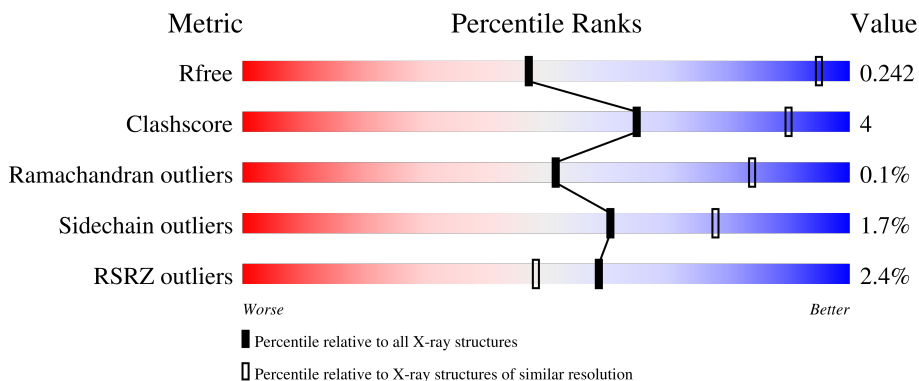
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



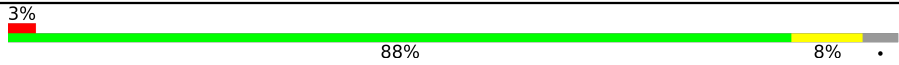

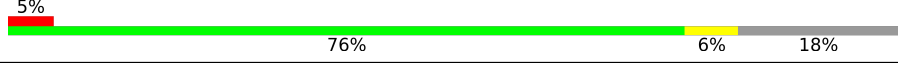
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	600	 90% 8%
1	B	600	 90% 9%
1	C	600	 85% 9% 6%
2	D	465	 84% 13%
2	E	465	 85% 12%

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Mol	Chain	Length	Quality of chain
2	F	465	 <p>3% 88% 8%</p>
3	G	217	 <p>7% 71% 24%</p>
4	H	115	 <p>5% 76% 6% 18%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23655 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	588	4197	2648	694	829	3	23	0	0	0
1	B	593	4250	2661	710	853	3	23	0	0	0
1	C	563	3924	2461	665	772	3	23	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	452	Total	C	N	O	Se	0	0	0
			3181	2021	544	602	14			
2	E	452	Total	C	N	O	Se	0	0	0
			3352	2123	562	653	14			
2	F	448	Total	C	N	O	Se	0	0	0
			3097	1954	524	604	15			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637

- Molecule 3 is a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	G	164	Total	C	N	O	S	Se	0	0	0
			1081	677	187	207	1	9			

- Molecule 4 is a protein called V-type sodium ATPase subunit G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
4	H	94	Total	C	N	O	S	Se	0	0	0
			573	360	99	112	1	1			

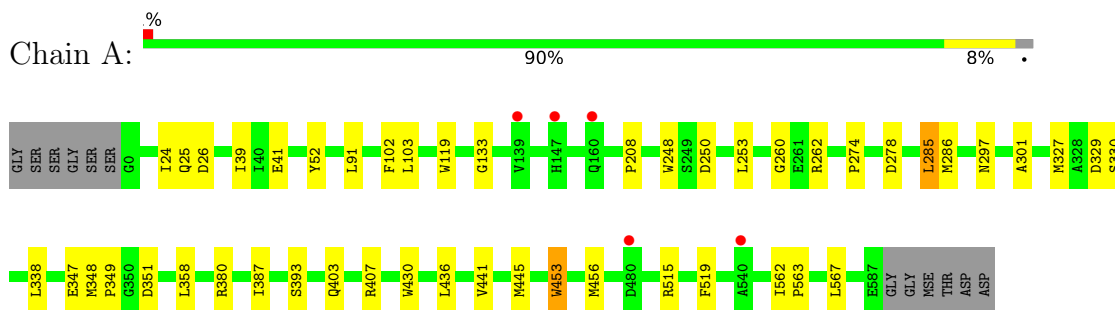
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP P43455
H	105	GLY	-	expression tag	UNP P43455
H	106	PRO	-	expression tag	UNP P43455
H	107	SER	-	expression tag	UNP P43455
H	108	SER	-	expression tag	UNP P43455
H	109	GLY	-	expression tag	UNP P43455
H	110	GLU	-	expression tag	UNP P43455
H	111	ASN	-	expression tag	UNP P43455
H	112	LEU	-	expression tag	UNP P43455
H	113	TYR	-	expression tag	UNP P43455
H	114	PHE	-	expression tag	UNP P43455
H	115	GLN	-	expression tag	UNP P43455

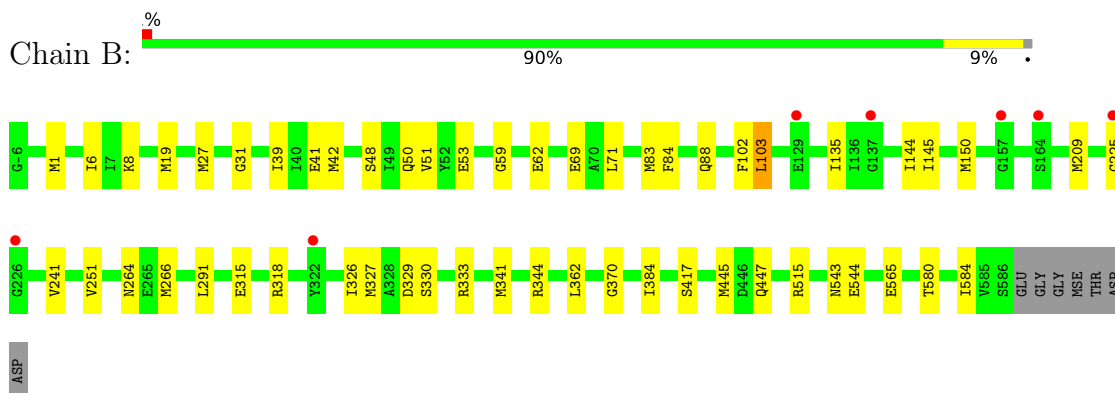
3 Residue-property plots

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.

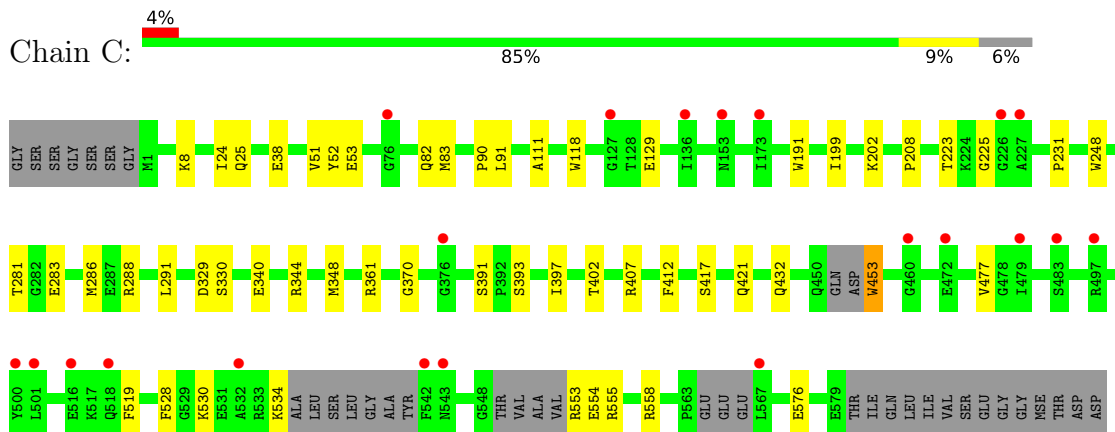
- Molecule 1: V-type sodium ATPase catalytic subunit A



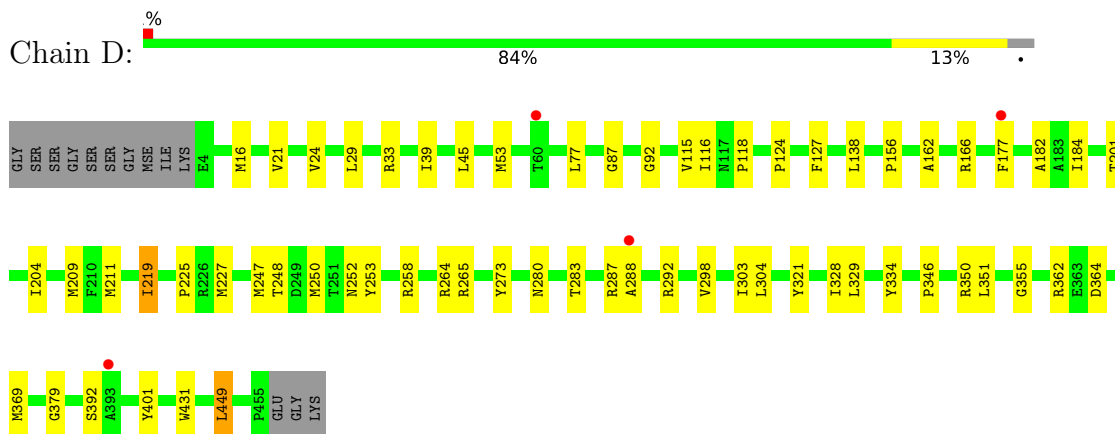
- Molecule 1: V-type sodium ATPase catalytic subunit A



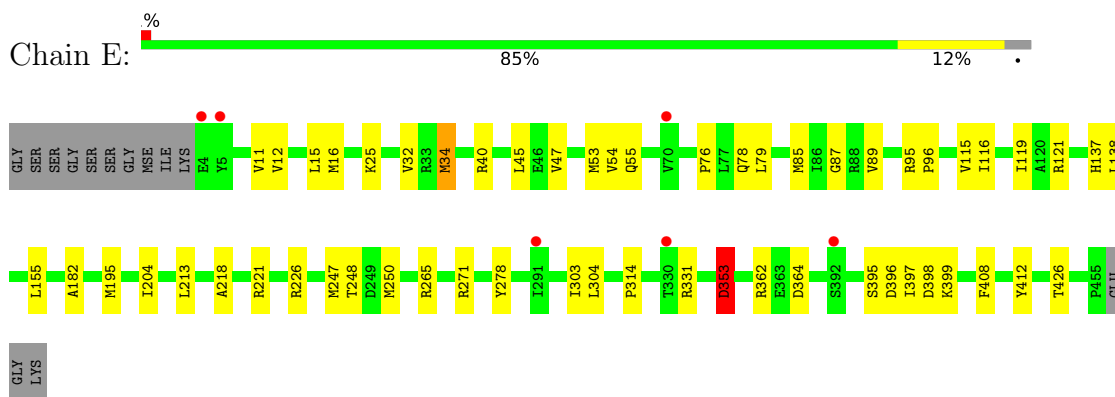
- Molecule 1: V-type sodium ATPase catalytic subunit A



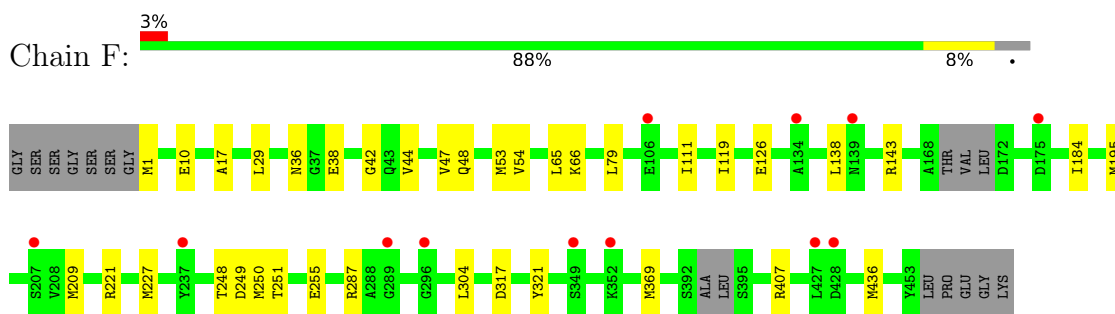
- Molecule 2: V-type sodium ATPase subunit B



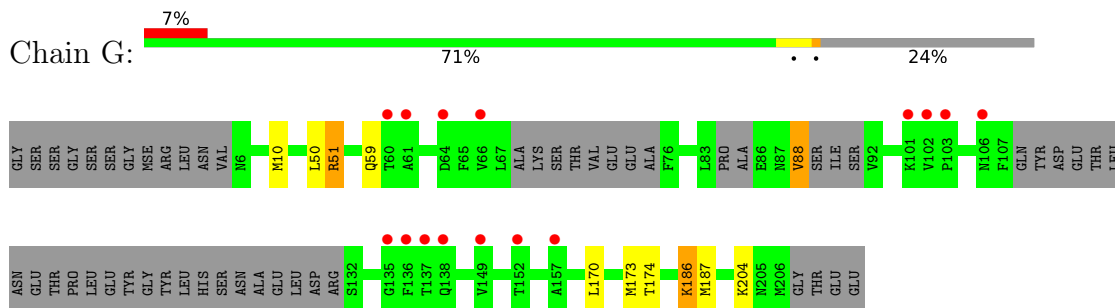
- Molecule 2: V-type sodium ATPase subunit B



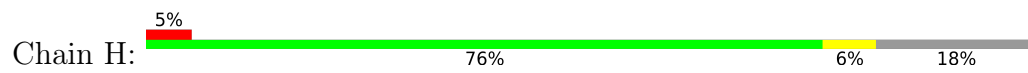
- Molecule 2: V-type sodium ATPase subunit B



- Molecule 3: V-type sodium ATPase subunit D



- Molecule 4: V-type sodium ATPase subunit G



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.33Å 129.32Å 234.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.90 49.60 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.60-3.90) 97.9 (49.60-3.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.250 0.208 , 0.242	Depositor DCC
R_{free} test set	1806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	101.5	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 135.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.150 for k,h,-l	Xtriage
Reported twinning fraction	0.767 for H, K, L 0.233 for K, H, -L	Depositor
Outliers	0 of 36120 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23655	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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	0.72	4/4248 (0.1%)	0.77	5/5769 (0.1%)
1	B	0.75	0/4297	0.79	4/5827 (0.1%)
1	C	0.68	4/3967 (0.1%)	0.71	0/5382
2	D	0.63	1/3226 (0.0%)	0.73	1/4395 (0.0%)
2	E	0.76	0/3400	0.82	3/4611 (0.1%)
2	F	0.66	0/3134	0.73	0/4264
3	G	0.56	0/1076	0.72	1/1456 (0.1%)
4	H	0.45	0/576	0.53	0/792
All	All	0.69	9/23924 (0.0%)	0.75	14/32496 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	TRP	CD2-CE2	6.17	1.48	1.41
2	D	431	TRP	CD2-CE2	5.93	1.48	1.41
1	C	248	TRP	CD2-CE2	5.59	1.48	1.41
1	A	430	TRP	CD2-CE2	5.30	1.47	1.41
1	A	248	TRP	CD2-CE2	5.30	1.47	1.41
1	A	453	TRP	CD2-CE2	5.28	1.47	1.41
1	C	118	TRP	CD2-CE2	5.21	1.47	1.41
1	A	119	TRP	CD2-CE2	5.12	1.47	1.41
1	C	453	TRP	CD2-CE2	5.02	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	353	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	456	MSE	CG-SE-CE	6.64	113.51	98.90
1	A	250	ASP	CB-CG-OD2	-6.36	112.58	118.30
2	E	226	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	E	213	LEU	CB-CG-CD1	5.86	120.97	111.00
1	B	344	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	D	292	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ASP	CB-CG-OD2	-5.40	113.44	118.30
3	G	173	MSE	CB-CG-SE	-5.32	96.74	112.70
1	A	278	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	362	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	B	241	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	A	358	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	B	318	ARG	NE-CZ-NH1	5.00	122.80	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	4197	0	3871	31	0
1	B	4250	0	3928	37	0
1	C	3924	0	3525	32	0
2	D	3181	0	2919	41	0
2	E	3352	0	3171	40	0
2	F	3097	0	2766	25	0
3	G	1081	0	910	11	0
4	H	573	0	467	6	0
All	All	23655	0	21557	186	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 (186) 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:83:MSE:HG3	1:B:291:LEU:CD1	1.49	1.43
2:F:407:ARG:HH11	2:F:436:MSE:SE	1.58	1.37
1:B:83:MSE:CG	1:B:291:LEU:HD11	1.69	1.21
2:F:407:ARG:NH1	2:F:436:MSE:SE	2.35	1.08
3:G:51:ARG:NH2	4:H:75:LEU:O	1.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:396:ASP:O	2:E:399:LYS:N	1.98	0.95
2:F:407:ARG:HD3	2:F:436:MSE:SE	2.23	0.88
1:B:83:MSE:HG3	1:B:291:LEU:HD11	0.89	0.88
2:D:45:LEU:HB2	2:D:53:MSE:HE3	1.63	0.80
1:B:83:MSE:CG	1:B:291:LEU:CD1	2.42	0.79
3:G:59:GLN:OE1	4:H:81:GLY:HA2	1.83	0.79
2:F:79:LEU:HD13	2:F:227:MSE:HE1	1.65	0.78
1:B:333:ARG:HD2	2:E:278:TYR:CE2	2.21	0.76
1:A:262:ARG:NH2	2:D:350:ARG:NH2	2.37	0.72
1:B:102:PHE:HE1	2:E:116:ILE:HG12	1.54	0.71
2:F:195:MSE:HE1	2:F:209:MSE:SE	2.41	0.71
1:B:50:GLN:HG3	1:B:341:MSE:HE3	1.73	0.69
1:C:391:SER:HB3	2:F:321:TYR:CE1	2.28	0.68
1:B:102:PHE:CE1	2:E:116:ILE:HG12	2.30	0.67
1:B:83:MSE:CB	1:B:291:LEU:HD11	2.25	0.66
1:B:543:ASN:OD1	1:B:544:GLU:N	2.29	0.66
3:G:186:LYS:O	3:G:186:LYS:HD2	1.95	0.66
2:E:182:ALA:HB3	2:E:247:MSE:HG2	1.79	0.65
1:A:445:MSE:HE1	1:A:515:ARG:HG3	1.78	0.65
1:C:83:MSE:SE	2:F:119:ILE:HG12	2.47	0.64
2:D:362:ARG:HD2	2:D:364:ASP:OD1	1.97	0.64
1:C:24:ILE:HG22	1:C:25:GLN:HG2	1.79	0.63
1:A:133:GLY:O	1:A:380:ARG:NH2	2.23	0.62
2:D:182:ALA:HB3	2:D:247:MSE:HG2	1.80	0.62
2:E:34:MSE:HE1	2:E:40:ARG:HG3	1.80	0.62
1:B:83:MSE:HE1	1:B:266:MSE:HB3	1.82	0.61
1:B:42:MSE:HG2	2:F:65:LEU:HD13	1.82	0.61
2:F:10:GLU:HG2	2:F:17:ALA:HB3	1.82	0.61
1:A:297:ASN:ND2	2:D:115:VAL:HG13	2.17	0.60
2:E:396:ASP:O	2:E:398:ASP:N	2.35	0.59
1:B:19:MSE:HE3	1:B:39:ILE:HD11	1.85	0.59
1:C:51:VAL:HG12	1:C:53:GLU:H	1.68	0.58
2:F:36:ASN:HD21	2:F:38:GLU:CD	2.06	0.58
1:B:144:ILE:HG23	1:B:145:ILE:N	2.19	0.57
2:D:53:MSE:HE1	2:D:264:ARG:HG2	1.87	0.57
2:E:11:VAL:HG22	2:E:16:MSE:HG3	1.86	0.57
2:F:184:ILE:HG22	2:F:221:ARG:HD2	1.87	0.57
2:E:362:ARG:HD2	2:E:364:ASP:OD1	2.05	0.57
1:B:445:MSE:HE1	1:B:515:ARG:HG3	1.87	0.56
1:A:393:SER:OG	2:D:321:TYR:OH	2.16	0.56
1:B:102:PHE:CD1	2:E:116:ILE:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:186:LYS:O	3:G:186:LYS:CD	2.54	0.56
1:C:83:MSE:HG2	1:C:91:LEU:HD12	1.87	0.55
1:C:348:MSE:HE1	3:G:204:LYS:HA	1.88	0.55
1:A:327:MSE:HG2	1:A:387:ILE:HB	1.88	0.55
2:E:395:SER:O	2:E:396:ASP:C	2.43	0.55
1:B:135:ILE:HD13	1:B:150:MSE:HG2	1.88	0.55
2:E:76:PRO:O	2:E:78:GLN:HG3	2.08	0.54
2:E:396:ASP:O	2:E:397:ILE:C	2.46	0.54
2:E:79:LEU:HD21	2:E:85:MSE:HE1	1.89	0.53
2:D:328:ILE:HD12	2:D:346:PRO:HB2	1.91	0.52
1:A:91:LEU:HD13	2:D:118:PRO:HG2	1.91	0.52
1:C:286:MSE:HE1	1:C:291:LEU:HD12	1.91	0.52
2:D:250:MSE:HB2	2:D:304:LEU:HB3	1.91	0.52
1:B:83:MSE:HG3	1:B:291:LEU:HD12	1.73	0.52
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.92	0.52
3:G:51:ARG:HD3	4:H:87:LEU:HG	1.91	0.52
1:C:412:PHE:HE2	1:C:432:GLN:HG2	1.74	0.52
2:D:138:LEU:HD23	2:D:369:MSE:HG3	1.92	0.51
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.92	0.51
2:E:16:MSE:HE1	2:E:32:VAL:CG2	2.41	0.51
1:C:8:LYS:HG3	2:F:48:GLN:HB3	1.91	0.51
1:B:83:MSE:CE	1:B:266:MSE:HB3	2.40	0.51
1:C:83:MSE:SE	2:F:119:ILE:CG1	3.09	0.50
1:A:26:ASP:HB2	1:A:39:ILE:HD12	1.92	0.50
2:F:111:ILE:O	2:F:287:ARG:NH2	2.40	0.50
2:F:138:LEU:HA	2:F:369:MSE:HG3	1.94	0.50
1:C:530:LYS:O	1:C:534:LYS:HG2	2.12	0.50
1:A:347:GLU:HA	2:E:265:ARG:NH2	2.27	0.50
2:E:45:LEU:HD11	2:E:55:GLN:HB2	1.94	0.50
1:B:41:GLU:HB2	1:B:48:SER:HB2	1.93	0.49
2:D:127:PHE:HB2	2:D:355:GLY:O	2.13	0.49
1:B:102:PHE:HD1	2:E:116:ILE:HA	1.77	0.49
1:C:555:ARG:NH1	1:C:576:GLU:OE2	2.42	0.49
1:C:199:ILE:HD11	1:C:202:LYS:HG3	1.94	0.49
2:D:184:ILE:HD13	2:D:225:PRO:HG3	1.94	0.49
2:D:29:LEU:HD21	2:D:77:LEU:HG	1.94	0.49
1:A:297:ASN:HD22	2:D:115:VAL:HG22	1.78	0.49
1:A:208:PRO:HG3	1:A:441:VAL:HG22	1.95	0.48
4:H:77:PRO:HB3	4:H:82:THR:HG22	1.94	0.48
1:A:41:GLU:OE1	2:E:12:VAL:HG13	2.13	0.48
2:E:34:MSE:HE1	2:E:40:ARG:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:ARG:HD2	2:D:273:TYR:CE2	2.48	0.48
3:G:59:GLN:CD	4:H:81:GLY:HA2	2.34	0.48
2:E:16:MSE:HE2	2:E:54:VAL:HG21	1.96	0.48
2:D:21:VAL:HB	2:D:24:VAL:HG21	1.96	0.48
2:D:248:THR:HB	2:D:303:ILE:HB	1.96	0.47
2:D:283:THR:O	2:D:287:ARG:HG3	2.13	0.47
1:C:90:PRO:HD3	1:C:111:ALA:HA	1.96	0.47
2:D:449:LEU:H	2:D:449:LEU:HD23	1.78	0.47
1:C:397:ILE:HB	1:C:402:THR:HG21	1.97	0.47
2:E:155:LEU:HD21	2:E:331:ARG:HD3	1.97	0.47
1:C:340:GLU:OE1	1:C:344:ARG:NE	2.40	0.47
1:C:281:THR:HG22	1:C:283:GLU:HG2	1.96	0.46
1:A:348:MSE:HG3	2:E:265:ARG:HA	1.97	0.46
1:B:6:ILE:HD12	1:B:62:GLU:HB2	1.96	0.46
1:C:199:ILE:HD11	1:C:202:LYS:CG	2.46	0.46
2:F:407:ARG:HD3	2:F:436:MSE:CE	2.45	0.46
1:B:51:VAL:HG12	1:B:53:GLU:H	1.81	0.46
2:D:209:MSE:HE2	2:D:211:MSE:SE	2.66	0.46
2:E:353:ASP:OD1	2:E:353:ASP:N	2.45	0.46
1:B:59:GLY:HA3	2:E:25:LYS:HD3	1.98	0.46
2:E:395:SER:O	2:E:396:ASP:O	2.34	0.46
1:A:297:ASN:HD21	2:D:115:VAL:HG13	1.81	0.46
1:C:407:ARG:NH1	2:D:252:ASN:OD1	2.49	0.46
1:B:315:GLU:HA	1:B:384:ILE:HD11	1.97	0.46
1:C:348:MSE:HE3	2:D:265:ARG:HB3	1.98	0.46
2:E:89:VAL:HG21	2:E:195:MSE:HE1	1.98	0.46
2:E:271:ARG:CD	3:G:187:MSE:HE1	2.46	0.46
1:B:84:PHE:HB3	1:B:88:GLN:HA	1.98	0.45
1:C:393:SER:OG	2:F:317:ASP:OD2	2.25	0.45
2:D:45:LEU:CB	2:D:53:MSE:HE3	2.41	0.45
2:D:253:TYR:OH	2:D:280:ASN:OD1	2.12	0.45
4:H:23:ASP:OD1	4:H:25:GLN:NE2	2.42	0.45
1:C:199:ILE:CD1	1:C:202:LYS:HG2	2.47	0.45
1:C:329:ASP:HA	1:C:330:SER:HA	1.69	0.45
3:G:88:VAL:O	3:G:88:VAL:HG12	2.16	0.45
1:B:580:THR:O	1:B:584:ILE:HG13	2.17	0.45
1:A:262:ARG:CZ	2:D:350:ARG:CZ	2.95	0.45
2:D:288:ALA:HA	2:D:298:VAL:HB	1.99	0.45
1:B:31:GLY:HA2	1:B:62:GLU:HB3	1.99	0.44
1:B:103:LEU:HB2	2:E:115:VAL:HB	1.98	0.44
1:B:329:ASP:HA	1:B:330:SER:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:227:MSE:HE3	2:F:227:MSE:HB3	1.65	0.44
2:F:79:LEU:HD13	2:F:227:MSE:CE	2.41	0.44
1:A:262:ARG:NH2	2:D:350:ARG:CZ	2.80	0.44
2:E:408:PHE:O	2:E:412:TYR:HB3	2.18	0.44
1:B:209:MSE:HE2	1:B:251:VAL:CG1	2.48	0.44
2:E:248:THR:HB	2:E:303:ILE:HB	1.98	0.44
1:C:208:PRO:HA	1:C:223:THR:HA	1.99	0.44
3:G:186:LYS:CD	3:G:186:LYS:C	2.86	0.44
1:B:144:ILE:CG2	1:B:145:ILE:N	2.80	0.44
1:C:361:ARG:HD3	1:C:361:ARG:HA	1.85	0.44
2:F:251:THR:O	2:F:255:GLU:HG2	2.17	0.44
1:C:453:TRP:CZ3	1:C:519:PHE:HA	2.53	0.43
2:D:124:PRO:HG2	2:D:351:LEU:HD13	2.00	0.43
2:F:29:LEU:HD12	2:F:42:GLY:O	2.18	0.43
1:A:274:PRO:HA	1:A:286:MSE:HG2	1.98	0.43
2:E:87:GLY:HA2	2:E:204:ILE:O	2.18	0.43
2:D:87:GLY:HA2	2:D:204:ILE:O	2.19	0.43
1:A:453:TRP:CZ3	1:A:519:PHE:HA	2.54	0.43
1:C:225:GLY:O	1:C:370:GLY:HA2	2.18	0.43
1:A:262:ARG:HH22	2:D:350:ARG:NH2	2.16	0.43
1:A:348:MSE:HE3	1:A:349:PRO:HD2	2.01	0.43
1:B:27:MSE:SE	1:B:71:LEU:HB2	2.69	0.43
1:A:297:ASN:ND2	2:D:115:VAL:HG22	2.33	0.43
1:A:329:ASP:HA	1:A:330:SER:HA	1.61	0.43
2:D:219:ILE:H	2:D:219:ILE:HG12	1.48	0.43
1:B:8:LYS:HA	2:E:47:VAL:O	2.19	0.43
2:E:218:ALA:HA	2:E:221:ARG:HG3	2.01	0.43
2:F:126:GLU:OE1	2:F:143:ARG:HD2	2.18	0.42
1:C:528:PHE:CZ	1:C:553:ARG:HD3	2.54	0.42
1:A:52:TYR:CD2	1:A:301:ALA:HB2	2.54	0.42
1:A:403:GLN:O	1:A:407:ARG:HG3	2.19	0.42
1:A:102:PHE:HE1	2:D:116:ILE:HG12	1.85	0.42
2:D:162:ALA:O	2:D:166:ARG:HB2	2.20	0.42
2:F:250:MSE:HB2	2:F:304:LEU:HB3	2.01	0.42
3:G:170:LEU:HA	3:G:174:THR:HB	2.00	0.42
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.81	0.42
1:C:38:GLU:OE1	1:C:52:TYR:OH	2.29	0.42
2:D:379:GLY:HA2	2:D:401:TYR:HB3	2.02	0.42
2:E:16:MSE:HE1	2:E:32:VAL:HG21	2.01	0.41
2:E:250:MSE:HB2	2:E:304:LEU:HB3	2.02	0.41
2:F:248:THR:HA	2:F:249:ASP:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:OD1	2:E:121:ARG:HD3	2.19	0.41
2:E:137:HIS:HB2	2:E:426:THR:HG21	2.02	0.41
1:B:543:ASN:OD1	1:B:543:ASN:C	2.58	0.41
1:A:562:ILE:HA	1:A:563:PRO:HD3	1.89	0.41
1:C:554:GLU:OE2	1:C:558:ARG:NH2	2.54	0.41
1:C:231:PRO:HG2	1:C:412:PHE:HE1	1.86	0.41
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.94	0.41
1:A:453:TRP:HZ3	1:A:519:PHE:HA	1.86	0.41
1:B:225:GLY:O	1:B:370:GLY:HA2	2.20	0.41
2:E:247:MSE:HE3	2:E:247:MSE:HB2	1.95	0.41
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.56	0.41
2:D:33:ARG:HA	2:D:39:ILE:HD13	2.03	0.40
2:D:92:GLY:O	2:D:227:MSE:HG3	2.21	0.40
2:E:95:ARG:HA	2:E:96:PRO:HD3	1.95	0.40
2:F:44:VAL:HA	2:F:54:VAL:HG12	2.01	0.40
1:C:417:SER:O	1:C:421:GLN:HG3	2.22	0.40
1:A:441:VAL:O	1:A:445:MSE:HG2	2.21	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	586/600 (98%)	573 (98%)	12 (2%)	1 (0%)	47 79
1	B	591/600 (98%)	581 (98%)	10 (2%)	0	100 100
1	C	553/600 (92%)	539 (98%)	13 (2%)	1 (0%)	47 79
2	D	450/465 (97%)	435 (97%)	15 (3%)	0	100 100
2	E	450/465 (97%)	436 (97%)	14 (3%)	0	100 100
2	F	442/465 (95%)	432 (98%)	10 (2%)	0	100 100
3	G	154/217 (71%)	151 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	88/115 (76%)	87 (99%)	1 (1%)	0	100	100
All	All	3314/3527 (94%)	3234 (98%)	78 (2%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	477	VAL
1	A	260	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	412/487 (85%)	407 (99%)	5 (1%)	71	83
1	B	423/487 (87%)	415 (98%)	8 (2%)	57	75
1	C	367/487 (75%)	364 (99%)	3 (1%)	81	89
2	D	288/372 (77%)	282 (98%)	6 (2%)	53	73
2	E	331/372 (89%)	324 (98%)	7 (2%)	53	73
2	F	272/372 (73%)	268 (98%)	4 (2%)	65	80
3	G	85/188 (45%)	80 (94%)	5 (6%)	19	49
4	H	42/97 (43%)	42 (100%)	0	100	100
All	All	2220/2862 (78%)	2182 (98%)	38 (2%)	60	78

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

Mol	Chain	Res	Type
1	A	103	LEU
1	A	253	LEU
1	A	285	LEU
1	A	436	LEU
1	A	567	LEU
1	B	1	MSE

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Mol	Chain	Res	Type
1	B	69	GLU
1	B	103	LEU
1	B	326	ILE
1	B	327	MSE
1	B	417	SER
1	B	447	GLN
1	B	565	GLU
1	C	82	GLN
1	C	129	GLU
1	C	288	ARG
2	D	16	MSE
2	D	177	PHE
2	D	219	ILE
2	D	329	LEU
2	D	392	SER
2	D	449	LEU
2	E	15	LEU
2	E	34	MSE
2	E	53	MSE
2	E	119	ILE
2	E	138	LEU
2	E	314	PRO
2	E	353	ASP
2	F	1	MSE
2	F	47	VAL
2	F	53	MSE
2	F	66	LYS
3	G	10	MSE
3	G	50	LEU
3	G	51	ARG
3	G	88	VAL
3	G	186	LYS

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

Mol	Chain	Res	Type
1	C	82	GLN
2	F	48	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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	565/600 (94%)	-0.14	5 (0%) 84 77	51, 97, 159, 192	0
1	B	570/600 (95%)	-0.06	7 (1%) 79 70	54, 105, 152, 181	0
1	C	540/600 (90%)	0.14	21 (3%) 39 30	70, 123, 186, 221	0
2	D	438/465 (94%)	-0.07	4 (0%) 84 77	66, 109, 165, 185	0
2	E	438/465 (94%)	-0.15	6 (1%) 75 66	44, 84, 126, 169	0
2	F	433/465 (93%)	0.05	12 (2%) 53 41	66, 115, 193, 232	0
3	G	155/217 (71%)	0.23	15 (9%) 7 6	87, 126, 215, 381	0
4	H	93/115 (80%)	0.28	6 (6%) 18 13	149, 190, 267, 403	0
All	All	3232/3527 (91%)	-0.01	76 (2%) 59 48	44, 107, 181, 403	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	227	ALA	4.5
3	G	106	ASN	4.3
3	G	102	VAL	3.9
3	G	60	THR	3.7
2	E	4	GLU	3.7
4	H	95	GLU	3.6
2	F	296	GLY	3.5
2	E	330	THR	3.4
1	C	500	TYR	3.4
2	E	392	SER	3.4
2	E	5	TYR	3.2
1	C	226	GLY	3.1
3	G	157	ALA	3.1
3	G	135	GLY	3.1
3	G	64	ASP	3.0
4	H	100	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	543	ASN	2.9
1	C	472	GLU	2.9
3	G	61	ALA	2.9
1	A	540	ALA	2.8
2	E	291	ILE	2.8
1	C	76	GLY	2.8
1	B	157	GLY	2.8
1	C	376	GLY	2.7
4	H	94	VAL	2.7
4	H	46	GLY	2.7
1	C	460	GLY	2.7
1	C	501	LEU	2.7
2	F	349	SER	2.7
2	E	70	VAL	2.7
3	G	66	VAL	2.7
1	B	226	GLY	2.6
1	C	136	ILE	2.6
1	C	542	PHE	2.5
2	D	393	ALA	2.5
3	G	137	THR	2.5
3	G	136	PHE	2.5
2	F	289	GLY	2.5
1	B	322	TYR	2.4
2	F	175	ASP	2.4
1	C	567	LEU	2.4
1	C	497	ARG	2.4
1	C	127	GLY	2.4
3	G	103	PRO	2.4
1	A	480	ASP	2.4
1	C	518	GLN	2.4
2	D	177	PHE	2.3
4	H	96	LYS	2.3
3	G	149	VAL	2.3
2	D	60	THR	2.3
4	H	31	THR	2.3
3	G	138	GLN	2.3
1	C	153	ASN	2.3
2	D	288	ALA	2.3
1	A	147	HIS	2.3
2	F	237	TYR	2.2
1	C	483	SER	2.2
1	B	137	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLN	2.2
2	F	427	LEU	2.2
2	F	207	SER	2.2
2	F	352	LYS	2.1
1	B	164	SER	2.1
1	C	516	GLU	2.1
3	G	152	THR	2.1
1	C	532	ALA	2.1
1	C	173	ILE	2.1
2	F	428	ASP	2.1
3	G	101	LYS	2.1
1	A	139	VAL	2.1
1	C	479	ILE	2.0
1	B	225	GLY	2.0
2	F	139	ASN	2.0
1	B	129	GLU	2.0
2	F	134	ALA	2.0
2	F	106	GLU	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.