



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:26 AM UTC

PDB ID : 3VR5 / pdb_00003vr5
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

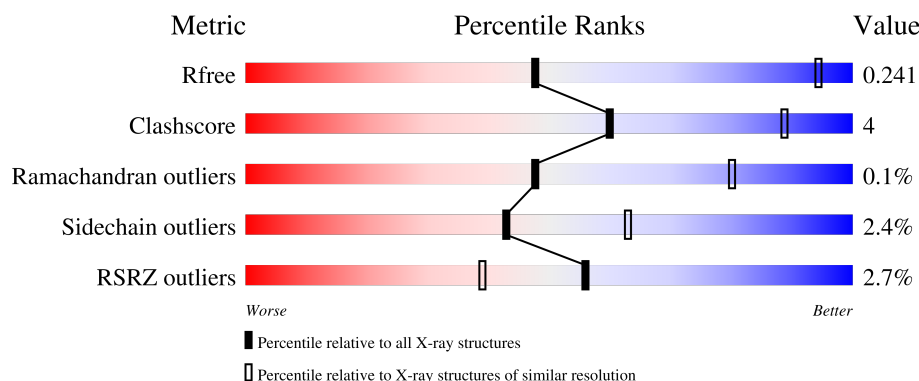
1 Overall quality at a glance

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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 90% 8% .
1	B	600	 % 89% 10% .
1	C	600	 4% 84% 9% 6%
2	D	465	 3% 83% 14% .
2	E	465	 2% 85% 11% ..

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Mol	Chain	Length	Quality of chain
2	F	465	3% 88% 8%
3	G	217	1% 70% 24%
4	H	115	7% 73% 9%

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
1	A	588	Total	C	N	O	S	Se	0	0	0
			4197	2648	694	829	3	23			
1	B	593	Total	C	N	O	S	Se	0	0	0
			4250	2661	710	853	3	23			
1	C	563	Total	C	N	O	S	Se	0	0	0
			3924	2461	665	772	3	23			

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			

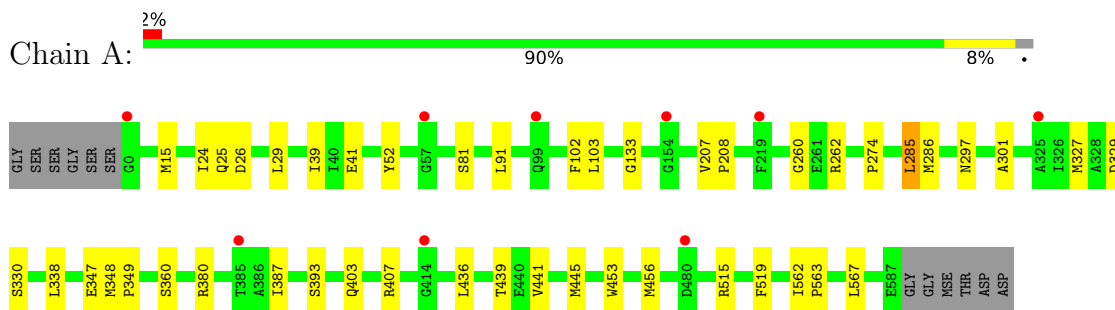
There are 12 discrepancies between the modelled and reference sequences:

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

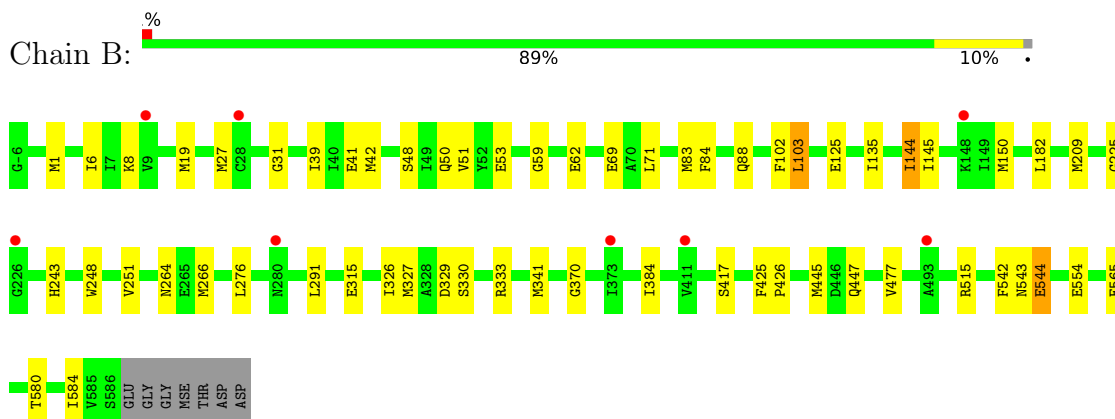
3 Residue-property plots [i](#)

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.

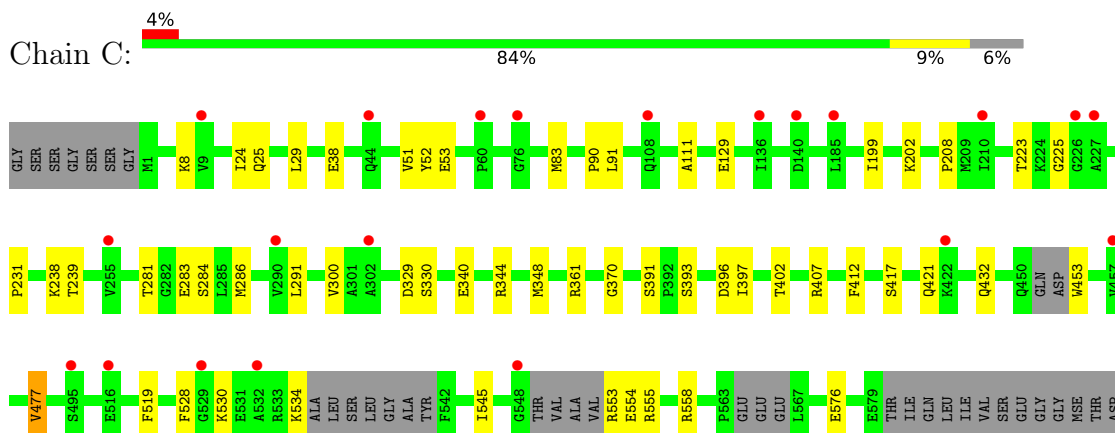
• Molecule 1: V-type sodium ATPase catalytic subunit A



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



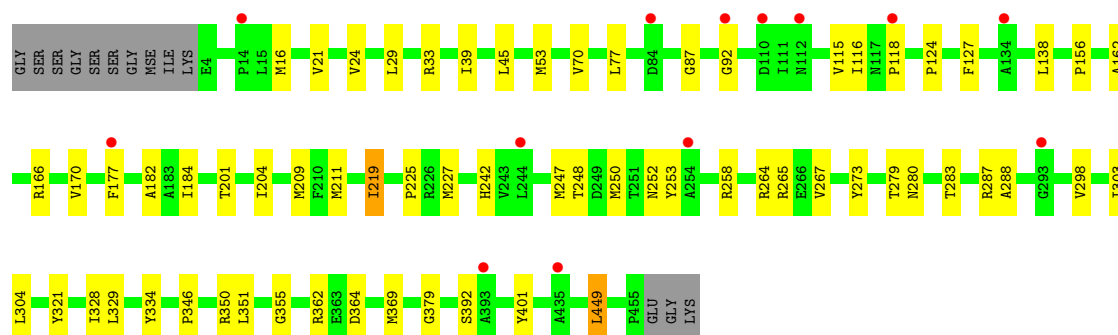
• Molecule 1: V-type sodium ATPase catalytic subunit A



ASP

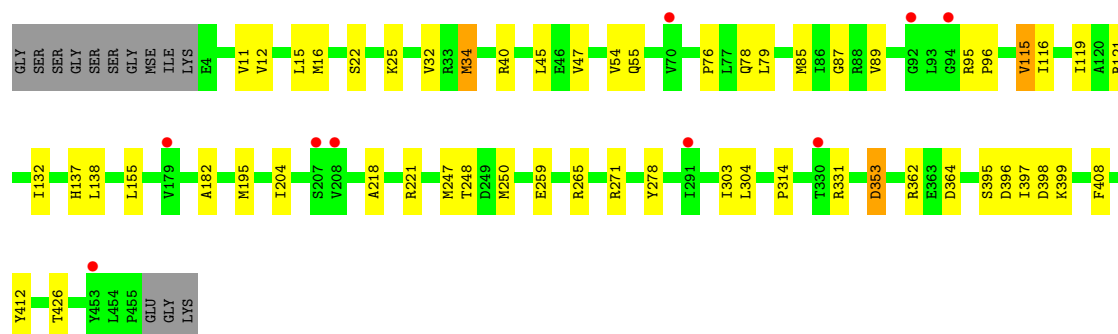
- Molecule 2: V-type sodium ATPase subunit B

Chain D:  3% 83% 14%



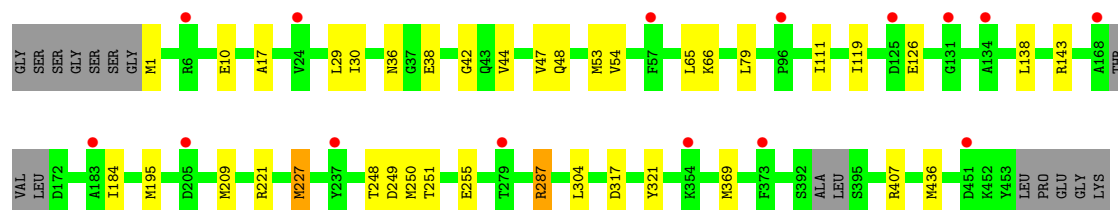
- Molecule 2: V-type sodium ATPase subunit B

Chain E:  2% 85% 11%



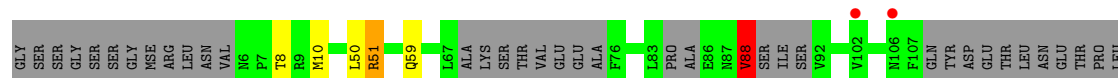
- Molecule 2: V-type sodium ATPase subunit B

Chain F:  3% 88% 8%



- Molecule 3: V-type sodium ATPase subunit D

Chain G:  0% 70% 24%





● Molecule 4: V-type sodium ATPase subunit G



4 Data and refinement statistics

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) 99.6 (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 0.207 , 0.241	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 , 167.8	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	0.86	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

5.1 Standard geometry

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	0.89	0/4248	1.02	2/5769 (0.0%)
1	B	0.95	1/4297 (0.0%)	1.03	4/5827 (0.1%)
1	C	0.87	2/3967 (0.1%)	1.01	4/5382 (0.1%)
2	D	0.86	2/3226 (0.1%)	1.00	1/4395 (0.0%)
2	E	0.96	0/3400	1.02	1/4611 (0.0%)
2	F	0.90	0/3134	0.99	0/4264
3	G	0.81	0/1076	1.04	2/1456 (0.1%)
4	H	0.68	0/576	0.93	0/792
All	All	0.90	5/23924 (0.0%)	1.01	14/32496 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	238	LYS	CA-C	6.09	1.60	1.52
2	D	242	HIS	CG-ND1	-5.89	1.31	1.38
2	D	242	HIS	CD2-NE2	-5.80	1.31	1.37
1	C	238	LYS	C-O	5.75	1.30	1.24
1	B	243	HIS	CG-CD2	5.71	1.42	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	THR	N-CA-C	10.54	122.35	111.07
1	B	248	TRP	N-CA-C	7.45	122.66	113.50
2	D	267	VAL	CB-CA-C	-7.34	104.11	110.94
1	C	545	ILE	N-CA-C	7.08	118.69	110.62
1	B	144	ILE	CB-CA-C	-7.07	103.98	110.91
1	B	544	GLU	N-CA-C	-6.95	103.70	111.28
1	A	456	MSE	CG-SE-CE	6.63	113.51	98.92
1	B	542	PHE	N-CA-C	6.42	118.85	111.02
3	G	88	VAL	N-CA-CB	-5.53	102.09	111.50
1	C	300	VAL	CB-CA-C	-5.44	105.01	111.97
1	A	207	VAL	CB-CA-C	-5.39	104.58	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	SER	N-CA-C	5.38	117.47	110.53
2	E	115	VAL	CB-CA-C	-5.37	104.17	111.15
3	G	173	MSE	CB-CG-SE	-5.32	96.74	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	33	0
1	B	4250	0	3928	39	0
1	C	3924	0	3525	33	0
2	D	3181	0	2919	41	0
2	E	3352	0	3171	41	0
2	F	3097	0	2766	25	0
3	G	1081	0	910	12	0
4	H	573	0	467	7	0
All	All	23655	0	21557	192	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 (192) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:36:ASN:HD21	2:F:38:GLU:CD	2.06	0.62
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:395:SER:O	2:E:396:ASP:C	2.43	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
2:E:396:ASP:O	2:E:397:ILE:C	2.46	0.59
1:C:51:VAL:HG12	1:C:53:GLU:H	1.68	0.58
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
1:B:144:ILE:HG23	1:B:145:ILE:N	2.19	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:79:LEU:HD21	2:E:85:MSE:HE1	1.89	0.53
3:G:59:GLN:CD	4:H:81:GLY:HA2	2.34	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
2:D:258:ARG:HD2	2:D:273:TYR:CE2	2.48	0.48
3:G:186:LYS:CD	3:G:186:LYS:C	2.86	0.48
2:E:16:MSE:HE2	2:E:54:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:360:SER:OG	2:E:259:GLU:OE1	2.26	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
1:B:543:ASN:OD1	1:B:543:ASN:C	2.58	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
2:F:227:MSE:HE3	2:F:227:MSE:HB3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:425:PHE:HA	1:B:426:PRO:C	2.42	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
1:B:291:LEU:HD12	1:B:291:LEU:C	2.44	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
1:C:396:ASP:CG	3:G:8:THR:HG21	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:248:THR:HA	2:F:249:ASP:HA	1.86	0.41
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:A:81:SER:OG	1:A:286:MSE:O	2.35	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
4:H:11:LYS:O	4:H:15:SER:OG	2.27	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/600 (98%)	573 (98%)	12 (2%)	1 (0%)	43	74
1	B	591/600 (98%)	581 (98%)	10 (2%)	0	100	100
1	C	553/600 (92%)	539 (98%)	13 (2%)	1 (0%)	43	74
2	D	450/465 (97%)	435 (97%)	15 (3%)	0	100	100
2	E	450/465 (97%)	436 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	442/465 (95%)	432 (98%)	10 (2%)	0	100	100
3	G	154/217 (71%)	151 (98%)	3 (2%)	0	100	100
4	H	88/115 (76%)	87 (99%)	1 (1%)	0	100	100
All	All	3314/3527 (94%)	3234 (98%)	78 (2%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	477	VAL
1	A	260	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/487 (85%)	405 (98%)	7 (2%)	53	68
1	B	423/487 (87%)	410 (97%)	13 (3%)	35	57
1	C	367/487 (75%)	364 (99%)	3 (1%)	73	77
2	D	288/372 (77%)	279 (97%)	9 (3%)	35	57
2	E	331/372 (89%)	323 (98%)	8 (2%)	43	63
2	F	272/372 (73%)	265 (97%)	7 (3%)	40	60
3	G	85/188 (45%)	80 (94%)	5 (6%)	18	44
4	H	42/97 (43%)	41 (98%)	1 (2%)	43	63
All	All	2220/2862 (78%)	2167 (98%)	53 (2%)	43	63

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MSE
1	A	29	LEU
1	A	103	LEU
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	436	LEU
1	A	439	THR
1	A	567	LEU
1	B	1	MSE
1	B	69	GLU
1	B	103	LEU
1	B	125	GLU
1	B	182	LEU
1	B	276	LEU
1	B	326	ILE
1	B	327	MSE
1	B	417	SER
1	B	447	GLN
1	B	477	VAL
1	B	554	GLU
1	B	565	GLU
1	C	29	LEU
1	C	129	GLU
1	C	477	VAL
2	D	16	MSE
2	D	70	VAL
2	D	170	VAL
2	D	177	PHE
2	D	219	ILE
2	D	279	THR
2	D	329	LEU
2	D	392	SER
2	D	449	LEU
2	E	15	LEU
2	E	22	SER
2	E	34	MSE
2	E	119	ILE
2	E	132	ILE
2	E	138	LEU
2	E	314	PRO
2	E	353	ASP
2	F	1	MSE
2	F	30	ILE
2	F	47	VAL
2	F	53	MSE
2	F	66	LYS
2	F	227	MSE

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Mol	Chain	Res	Type
2	F	287	ARG
3	G	10	MSE
3	G	50	LEU
3	G	51	ARG
3	G	88	VAL
3	G	186	LYS
4	H	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	B	153	ASN
1	B	421	GLN
1	C	153	ASN
1	C	403	GLN
1	C	574	ASN
2	D	67	ASN
2	D	139	ASN
2	D	410	ASN
2	F	36	ASN
2	F	48	GLN
2	F	55	GLN
2	F	167	GLN
3	G	26	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	565/600 (94%)	0.20	9 (1%) 70 49	51, 97, 159, 192	0
1	B	570/600 (95%)	0.25	8 (1%) 73 52	54, 105, 152, 181	0
1	C	540/600 (90%)	0.47	21 (3%) 43 31	70, 123, 186, 221	0
2	D	438/465 (94%)	0.27	13 (2%) 52 36	66, 109, 165, 185	0
2	E	438/465 (94%)	0.11	9 (2%) 63 44	44, 84, 126, 169	0
2	F	433/465 (93%)	0.37	15 (3%) 47 33	66, 115, 193, 232	0
3	G	155/217 (71%)	0.36	3 (1%) 66 46	87, 126, 215, 381	0
4	H	93/115 (80%)	0.72	8 (8%) 16 17	149, 190, 267, 403	0
All	All	3232/3527 (91%)	0.30	86 (2%) 56 39	44, 107, 181, 403	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	422	LYS	4.3
1	C	529	GLY	4.1
2	D	393	ALA	4.0
1	B	9	VAL	3.9
4	H	55	ALA	3.8
2	E	291	ILE	3.7
4	H	95	GLU	3.7
1	C	495	SER	3.5
2	F	96	PRO	3.4
4	H	12	ASP	3.4
1	C	548	GLY	3.2
4	H	66	LYS	3.2
1	C	227	ALA	3.0
1	C	136	ILE	3.0
3	G	102	VAL	3.0
1	C	532	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	140	ASP	2.9
4	H	94	VAL	2.9
1	B	493	ALA	2.8
2	E	179	VAL	2.8
2	E	70	VAL	2.8
1	A	480	ASP	2.7
4	H	99	GLY	2.7
2	F	24	VAL	2.7
2	D	134	ALA	2.6
2	F	134	ALA	2.6
1	B	148	LYS	2.5
1	C	516	GLU	2.5
1	A	385	THR	2.5
1	B	373	ILE	2.5
2	E	207	SER	2.5
4	H	71	PRO	2.5
2	D	177	PHE	2.5
2	D	254	ALA	2.5
1	A	0	GLY	2.5
1	C	9	VAL	2.5
1	C	290	VAL	2.5
2	F	373	PHE	2.4
1	B	411	VAL	2.4
2	D	293	GLY	2.4
3	G	106	ASN	2.4
2	F	57	PHE	2.4
2	F	125	ASP	2.4
2	E	453	TYR	2.4
1	B	226	GLY	2.4
2	F	354	LYS	2.4
2	D	118	PRO	2.3
2	E	94	GLY	2.3
2	F	6	ARG	2.3
1	A	325	ALA	2.3
1	C	302	ALA	2.3
1	C	44	GLN	2.3
2	F	183	ALA	2.3
2	D	110	ASP	2.3
2	D	112	ASN	2.2
2	D	435	ALA	2.2
2	F	237	TYR	2.2
1	C	457	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	185	LEU	2.2
2	D	14	PRO	2.2
2	E	208	VAL	2.2
1	C	226	GLY	2.2
2	E	92	GLY	2.2
2	F	131	GLY	2.2
2	E	330	THR	2.2
1	B	280	ASN	2.2
3	G	157	ALA	2.1
2	F	451	ASP	2.1
1	A	57	GLY	2.1
1	A	219	PHE	2.1
2	D	92	GLY	2.1
1	A	99	GLN	2.1
1	C	210	ILE	2.1
1	B	28	CYS	2.1
1	A	154	GLY	2.1
2	D	84	ASP	2.1
2	D	244	LEU	2.1
2	F	279	THR	2.1
1	C	108	GLN	2.1
1	C	255	VAL	2.1
1	A	414	GLY	2.0
2	F	205	ASP	2.0
1	C	76	GLY	2.0
1	C	60	PRO	2.0
2	F	168	ALA	2.0
4	H	54	CYS	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 oligosaccharides 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.