Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2024 – 11:05 PM EST

PDB ID	:	3MZL
Title	:	Sec13/Sec31 edge element, loop deletion mutant
Authors	:	Whittle, J.R.; Schwartz, T.U.
Deposited on	:	2010-05-12
Resolution	:	2.80 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:

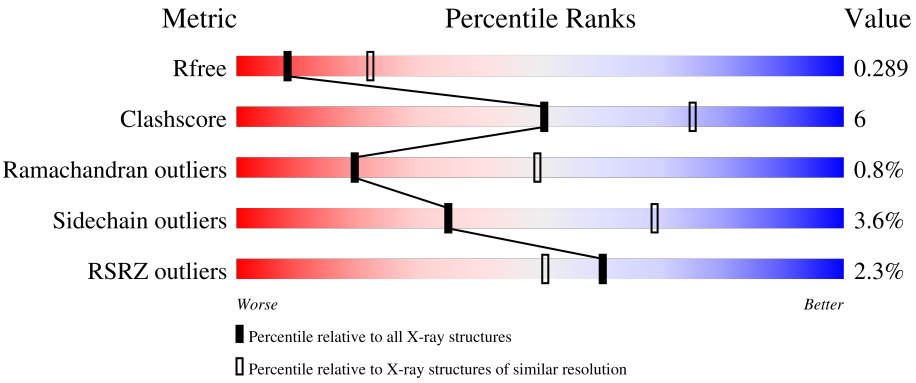
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	297	75% 18% · 6%
1	C	297	78% 15% · 6%
1	E	297	% 72% 21% · 6%
1	G	297	77% 17% 6%
2	B	345	6% 77% 18% · 5%

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Mol	Chain	Length	Quality of chain
2	D	345	3% 81% 14% 5%
2	F	345	2% 78% 18% 5%
2	H	345	4% 80% 15% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19212 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			
1	C	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			
1	E	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			
1	G	279	Total	C	N	O	S	0	0	0
			2196	1403	375	415	3			

- Molecule 2 is a protein called Protein transport protein SEC31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2607	1652	431	519	5			
2	D	329	Total	C	N	O	S	0	0	0
			2607	1652	431	519	5			
2	F	329	Total	C	N	O	S	0	0	0
			2607	1652	431	519	5			
2	H	329	Total	C	N	O	S	0	0	0
			2607	1652	431	519	5			

There are 8 discrepancies between the modelled and reference sequences:

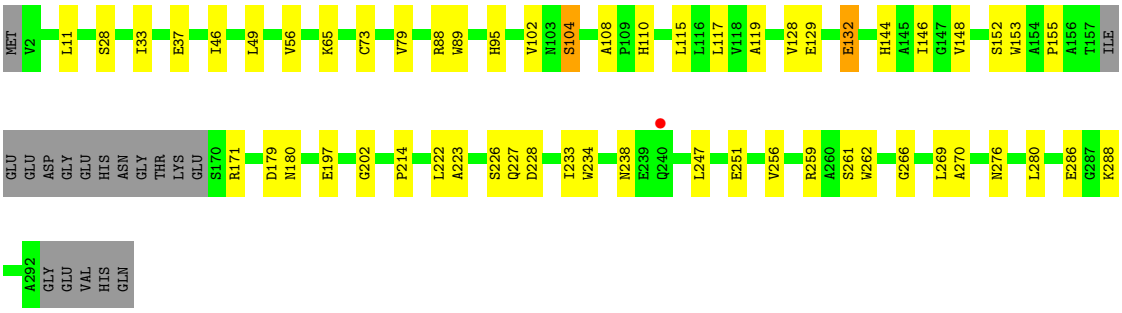
Chain	Residue	Modelled	Actual	Comment	Reference
B	368	GLY	-	expression tag	UNP P38968
B	369	PRO	-	expression tag	UNP P38968
D	368	GLY	-	expression tag	UNP P38968
D	369	PRO	-	expression tag	UNP P38968
F	368	GLY	-	expression tag	UNP P38968
F	369	PRO	-	expression tag	UNP P38968
H	368	GLY	-	expression tag	UNP P38968
H	369	PRO	-	expression tag	UNP P38968

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.

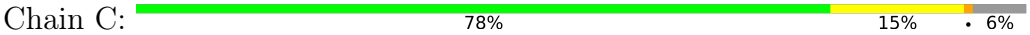
• Molecule 1: Protein transport protein SEC13

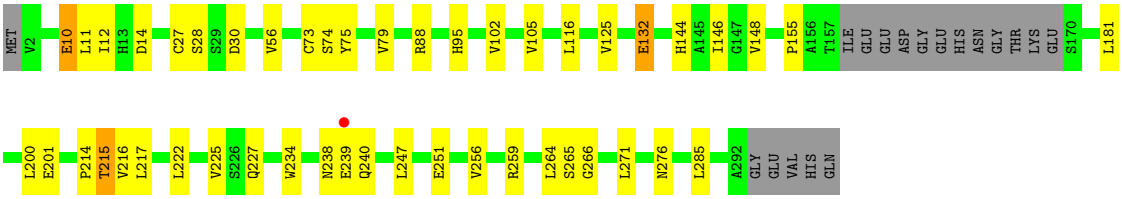
Chain A:



• Molecule 1: Protein transport protein SEC13

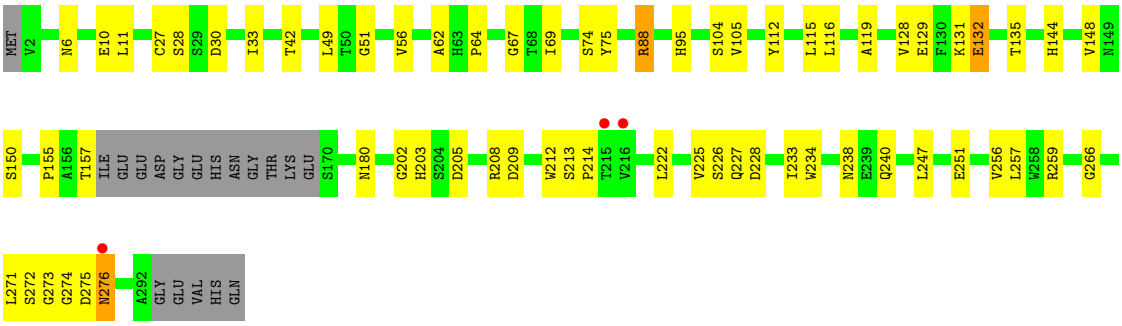
Chain C:





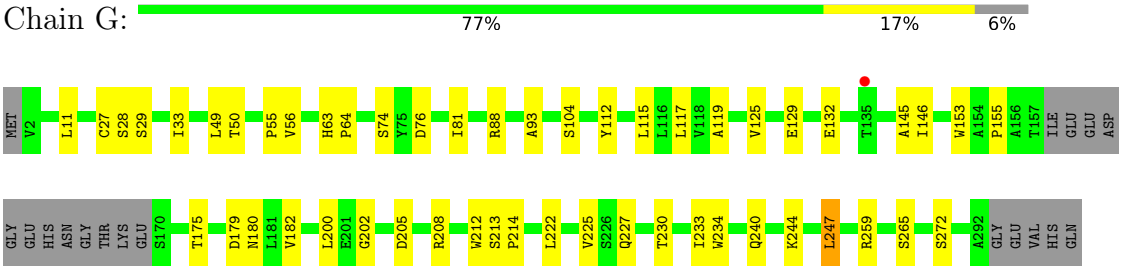
• Molecule 1: Protein transport protein SEC13

Chain E:



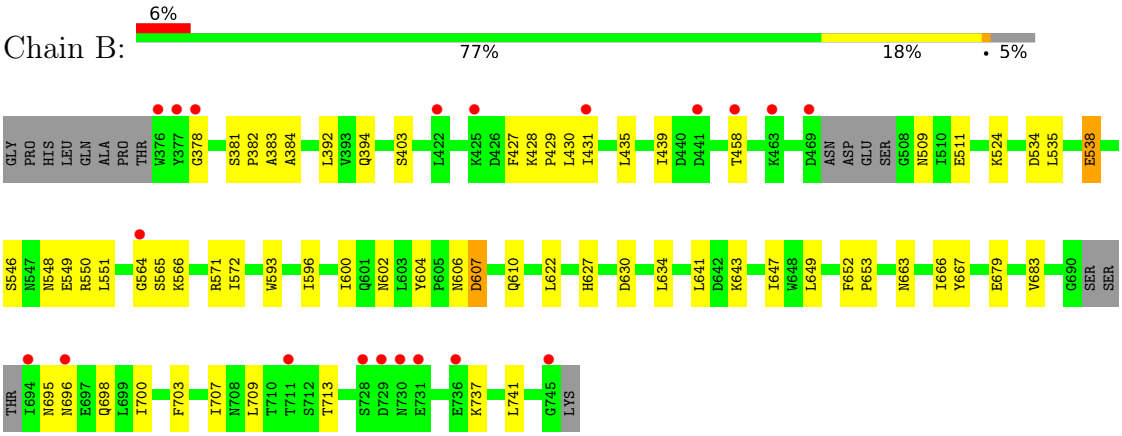
• Molecule 1: Protein transport protein SEC13

Chain G:



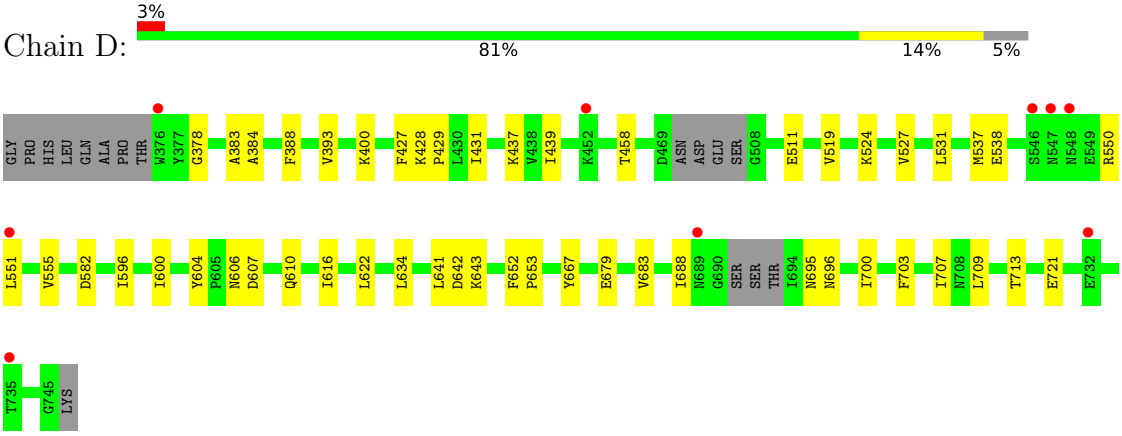
• Molecule 2: Protein transport protein SEC31

Chain B:



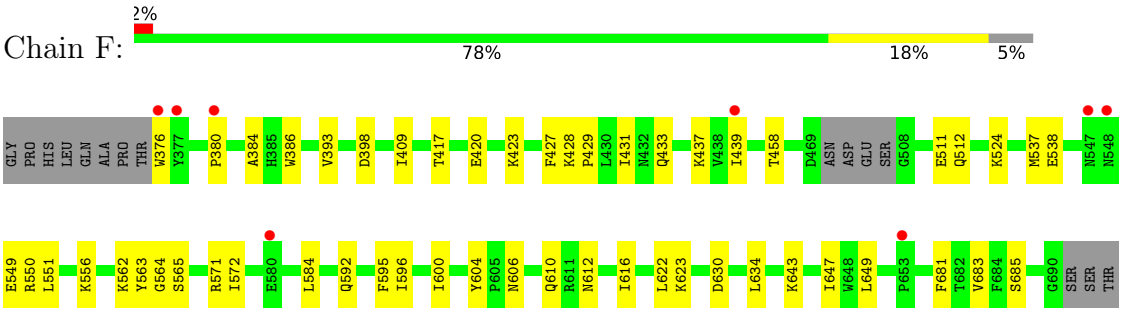
• Molecule 2: Protein transport protein SEC31

Chain D:

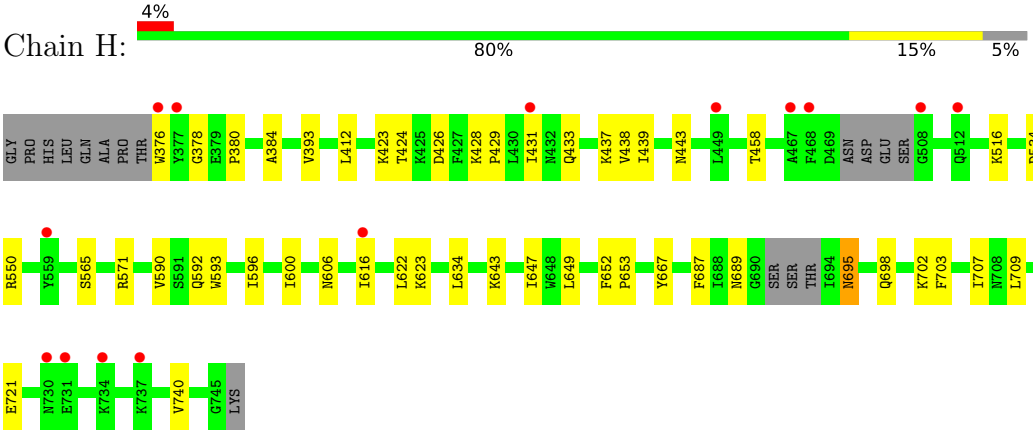


• Molecule 2: Protein transport protein SEC31

Chain F:



• Molecule 2: Protein transport protein SEC31



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	156.22Å 46.62Å 192.00Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	29.38 – 2.80 29.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.38-2.80) 83.4 (29.38-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.267 , 0.300 0.261 , 0.289	Depositor DCC
R_{free} test set	1792 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 8.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Reported twinning fraction	0.772 for H, K, L 0.228 for -h,-k,l	Depositor
Outliers	0 of 69354 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	19212	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2494e-03.*

[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

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	0.35	0/2256	0.53	0/3079
1	C	0.34	0/2256	0.52	0/3079
1	E	0.35	0/2256	0.52	0/3079
1	G	0.34	0/2256	0.51	0/3079
2	B	0.34	0/2647	0.49	0/3571
2	D	0.33	0/2647	0.48	0/3571
2	F	0.34	0/2647	0.48	0/3571
2	H	0.34	0/2647	0.48	0/3571
All	All	0.34	0/19612	0.50	0/26600

There are no bond length outliers.

There are no bond angle outliers.

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	2196	0	2138	29	0
1	C	2196	0	2138	24	0
1	E	2196	0	2138	38	0
1	G	2196	0	2138	29	0
2	B	2607	0	2601	33	0
2	D	2607	0	2601	25	0
2	F	2607	0	2601	32	0
2	H	2607	0	2601	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19212	0	18956	217	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 6.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:HB2	1:G:234:TRP:HB2	1.71	0.72
1:E:95:HIS:CE1	1:E:128:VAL:HG21	2.25	0.71
1:C:10:GLU:HG3	1:C:30:ASP:HB3	1.71	0.71
1:G:33:ILE:HD11	1:G:56:VAL:HG11	1.72	0.70
2:H:623:LYS:HD3	2:H:647:ILE:HD12	1.73	0.69
2:D:607:ASP:HA	1:E:42:THR:HG22	1.75	0.69
1:E:10:GLU:HG3	1:E:30:ASP:HB3	1.76	0.68
2:H:622:LEU:HD12	2:H:634:LEU:HD12	1.77	0.66
2:H:695:ASN:H	2:H:695:ASN:HD22	1.43	0.66
2:D:427:PHE:O	2:D:431:ILE:HG12	1.94	0.66
2:D:703:PHE:O	2:D:707:ILE:HG12	1.95	0.66
2:B:427:PHE:O	2:B:431:ILE:HG12	1.97	0.65
1:C:227:GLN:HA	1:C:256:VAL:HG13	1.78	0.64
1:G:33:ILE:CD1	1:G:56:VAL:HG11	2.27	0.64
1:A:261:SER:HB3	1:A:270:ALA:HB3	1.80	0.63
1:C:259:ARG:HG3	2:D:383:ALA:HA	1.79	0.63
1:C:27:CYS:HB2	1:C:56:VAL:HB	1.79	0.63
1:G:182:VAL:HB	1:G:200:LEU:HB2	1.80	0.63
2:B:596:ILE:O	2:B:600:ILE:HG12	2.00	0.62
2:F:649:LEU:HD13	2:F:698:GLN:HB3	1.81	0.62
2:F:433:GLN:O	2:F:437:LYS:HG2	1.99	0.62
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.14	0.61
1:C:222:LEU:HB2	1:C:234:TRP:HB2	1.82	0.61
1:E:112:TYR:HB3	1:E:115:LEU:HD12	1.82	0.61
2:F:713:THR:HG22	2:H:412:LEU:HD21	1.82	0.61
1:A:259:ARG:HG3	2:B:383:ALA:HA	1.83	0.60
2:H:428:LYS:HB2	2:H:429:PRO:HD3	1.84	0.59
2:F:683:VAL:HG11	2:H:431:ILE:HD11	1.83	0.59
1:C:155:PRO:HG3	1:C:214:PRO:HA	1.84	0.59
2:B:384:ALA:HB1	2:B:392:LEU:HD11	1.84	0.58
1:E:33:ILE:HB	1:E:49:LEU:HD12	1.85	0.58
2:H:695:ASN:HD22	2:H:695:ASN:N	2.02	0.58
2:F:524:LYS:HA	2:F:551:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:CYS:HB2	1:C:102:VAL:HG12	1.86	0.57
2:H:596:ILE:O	2:H:600:ILE:HG12	2.05	0.57
2:D:596:ILE:O	2:D:600:ILE:HG12	2.05	0.57
1:E:144:HIS:HB2	1:E:148:VAL:HG22	1.85	0.57
2:B:652:PHE:HB3	2:B:653:PRO:HD3	1.87	0.57
2:F:458:THR:HB	2:H:687:PHE:HB3	1.87	0.57
1:A:65:LYS:HE2	1:A:110:HIS:HB2	1.87	0.56
2:F:556:LYS:HG3	2:H:544:LEU:HD23	1.87	0.56
1:C:144:HIS:HB2	1:C:148:VAL:HG22	1.87	0.56
1:A:49:LEU:HD21	1:A:89:TRP:HB3	1.87	0.56
1:A:222:LEU:O	1:A:233:ILE:HA	2.06	0.55
2:B:622:LEU:HD12	2:B:634:LEU:HD12	1.87	0.55
1:E:227:GLN:HA	1:E:256:VAL:HG13	1.88	0.55
2:B:667:TYR:CZ	1:C:266:GLY:HA2	2.41	0.55
2:F:427:PHE:O	2:F:431:ILE:HG12	2.07	0.55
2:B:549:GLU:HG3	2:B:550:ARG:H	1.72	0.55
1:G:27:CYS:HB2	1:G:56:VAL:HB	1.88	0.54
1:G:11:LEU:O	1:G:28:SER:HB2	2.07	0.54
1:E:208:ARG:HH22	2:F:376:TRP:HA	1.72	0.54
1:G:155:PRO:HG3	1:G:214:PRO:HA	1.89	0.53
1:C:125:VAL:HG23	1:C:148:VAL:HG21	1.90	0.52
1:G:117:LEU:HB2	1:G:153:TRP:NE1	2.24	0.52
1:A:104:SER:HB3	1:A:119:ALA:HB3	1.90	0.52
2:F:622:LEU:HD12	2:F:634:LEU:HD12	1.92	0.52
1:G:230:THR:HB	1:G:247:LEU:HD21	1.92	0.52
2:B:649:LEU:HD13	2:B:698:GLN:HB3	1.92	0.52
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.91	0.51
1:E:222:LEU:HB2	1:E:234:TRP:HB2	1.91	0.51
1:E:266:GLY:HA2	2:H:667:TYR:CE1	2.45	0.51
2:D:709:LEU:O	2:D:713:THR:HG23	2.10	0.51
2:D:428:LYS:HB2	2:D:429:PRO:HD3	1.93	0.51
2:B:565:SER:HB2	2:B:571:ARG:NH2	2.26	0.50
1:E:203:HIS:ND1	1:E:226:SER:HB2	2.26	0.50
2:H:709:LEU:O	2:H:713:THR:HG23	2.12	0.50
2:H:652:PHE:HB3	2:H:653:PRO:HD3	1.92	0.50
2:B:524:LYS:HA	2:B:551:LEU:HD21	1.93	0.50
1:E:27:CYS:HB2	1:E:56:VAL:HB	1.93	0.50
2:B:430:LEU:HD21	2:D:679:GLU:HB3	1.94	0.50
2:B:643:LYS:O	2:B:647:ILE:HG12	2.12	0.50
2:D:524:LYS:HA	2:D:551:LEU:HD21	1.93	0.50
1:E:104:SER:HB3	1:E:119:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLN:HG2	2:B:403:SER:HB3	1.94	0.49
1:E:33:ILE:CD1	1:E:56:VAL:HG11	2.42	0.49
1:G:104:SER:HB3	1:G:119:ALA:HB3	1.93	0.49
2:F:562:LYS:HE2	2:F:563:TYR:CE1	2.48	0.49
1:E:222:LEU:O	1:E:233:ILE:HA	2.13	0.49
2:H:703:PHE:O	2:H:707:ILE:HG12	2.12	0.49
1:E:105:VAL:CG2	1:E:116:LEU:HD11	2.42	0.49
2:F:604:TYR:CZ	2:F:610:GLN:HG2	2.48	0.49
1:A:269:LEU:O	1:A:280:LEU:HA	2.13	0.49
2:B:602:ASN:ND2	2:D:519:VAL:O	2.45	0.49
2:H:433:GLN:O	2:H:437:LYS:HG2	2.13	0.49
2:B:627:HIS:HB3	2:B:630:ASP:HB2	1.94	0.49
1:A:266:GLY:HA2	2:D:667:TYR:CZ	2.48	0.48
1:A:155:PRO:HG3	1:A:214:PRO:HA	1.95	0.48
1:C:79:VAL:HB	1:C:95:HIS:HB3	1.95	0.48
2:D:616:ILE:HD12	2:D:643:LYS:HG3	1.94	0.48
1:E:257:LEU:HA	1:E:273:GLY:HA2	1.96	0.48
1:G:145:ALA:HB3	1:G:179:ASP:HB3	1.96	0.48
2:B:703:PHE:O	2:B:707:ILE:HG12	2.14	0.48
2:F:592:GLN:HB3	2:F:595:PHE:HD2	1.79	0.48
1:C:11:LEU:O	1:C:28:SER:HB2	2.14	0.47
2:F:623:LYS:HD3	2:F:647:ILE:HD12	1.97	0.47
1:G:29:SER:HA	1:G:55:PRO:HB3	1.96	0.47
1:G:112:TYR:HB3	1:G:115:LEU:HD12	1.97	0.47
2:B:431:ILE:HD11	2:D:683:VAL:HG11	1.97	0.47
2:B:696:ASN:O	2:B:700:ILE:HG12	2.14	0.47
1:E:155:PRO:HG3	1:E:214:PRO:HA	1.96	0.47
2:B:431:ILE:O	2:B:435:LEU:HB2	2.14	0.47
1:E:203:HIS:ND1	1:E:226:SER:CB	2.77	0.47
2:F:420:GLU:HA	2:F:423:LYS:HG2	1.97	0.47
1:G:115:LEU:HD23	1:G:129:GLU:HB2	1.97	0.47
1:A:79:VAL:HB	1:A:95:HIS:HB3	1.97	0.47
2:D:550:ARG:HE	1:E:88:ARG:HH12	1.61	0.47
2:D:652:PHE:HB3	2:D:653:PRO:HD3	1.96	0.47
1:E:259:ARG:HB2	1:E:272:SER:HB2	1.97	0.47
2:H:565:SER:HB2	2:H:571:ARG:NH2	2.30	0.47
1:C:14:ASP:HB3	1:C:27:CYS:SG	2.55	0.46
1:C:264:LEU:CD1	2:D:388:PHE:HA	2.46	0.46
2:F:622:LEU:CD1	2:F:634:LEU:HD12	2.45	0.46
2:H:423:LYS:HG3	2:H:424:THR:HG23	1.97	0.46
1:A:37:GLU:CG	1:A:46:ILE:HD11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:HB2	1:A:148:VAL:HG22	1.98	0.46
1:G:180:ASN:N	1:G:180:ASN:HD22	2.14	0.46
2:B:683:VAL:HG11	2:D:431:ILE:HD11	1.97	0.46
1:E:64:PRO:HA	1:E:67:GLY:O	2.16	0.46
1:A:222:LEU:HB2	1:A:234:TRP:HB2	1.97	0.46
1:E:180:ASN:N	1:E:180:ASN:HD22	2.14	0.46
2:D:641:LEU:HD21	2:D:688:ILE:HG21	1.98	0.46
2:F:428:LYS:HB2	2:F:429:PRO:HD3	1.97	0.46
1:G:81:ILE:HB	1:G:93:ALA:HB3	1.98	0.45
1:A:276:ASN:ND2	1:A:276:ASN:O	2.50	0.45
1:E:226:SER:OG	1:E:227:GLN:N	2.50	0.45
2:F:565:SER:HB2	2:F:571:ARG:NH2	2.32	0.45
1:G:125:VAL:HG21	1:G:175:THR:HG21	1.99	0.45
1:G:33:ILE:HB	1:G:49:LEU:HD12	1.97	0.45
1:G:200:LEU:HD13	1:G:234:TRP:CD2	2.51	0.45
1:A:108:ALA:HB2	1:A:153:TRP:CE2	2.51	0.45
1:A:115:LEU:HD11	1:A:171:ARG:NH1	2.32	0.45
2:H:438:VAL:HG23	2:H:443:ASN:HD22	1.82	0.45
1:A:223:ALA:HB2	1:A:262:TRP:CZ2	2.52	0.45
1:G:234:TRP:HA	1:G:244:LYS:O	2.17	0.45
2:B:428:LYS:HB2	2:B:429:PRO:HD3	1.98	0.44
1:C:105:VAL:HG22	1:C:116:LEU:HD11	1.98	0.44
1:G:259:ARG:HB2	1:G:272:SER:HB2	1.99	0.44
1:E:150:SER:CB	1:E:209:ASP:HA	2.46	0.44
1:A:33:ILE:CD1	1:A:56:VAL:HG11	2.47	0.44
2:F:596:ILE:O	2:F:600:ILE:HG12	2.17	0.44
2:H:384:ALA:HA	2:H:393:VAL:O	2.17	0.44
1:E:11:LEU:O	1:E:28:SER:HB2	2.18	0.44
1:E:274:GLY:C	1:E:276:ASN:H	2.21	0.44
1:G:213:SER:HA	1:G:214:PRO:HD3	1.86	0.44
2:B:666:ILE:HG22	1:C:217:LEU:HD13	2.00	0.44
1:G:63:HIS:HA	1:G:64:PRO:HD3	1.87	0.44
2:H:426:ASP:O	2:H:429:PRO:HD2	2.18	0.44
2:B:593:TRP:HA	2:B:596:ILE:HD12	1.99	0.43
2:B:679:GLU:O	2:B:683:VAL:HG23	2.17	0.43
1:C:200:LEU:HD13	1:C:234:TRP:CE3	2.53	0.43
1:E:205:ASP:HB3	1:E:227:GLN:HB3	2.00	0.43
2:H:549:GLU:O	2:H:550:ARG:HB2	2.17	0.43
1:A:115:LEU:HD23	1:A:129:GLU:HB2	2.00	0.43
1:E:226:SER:HB3	1:E:228:ASP:OD1	2.19	0.43
1:E:115:LEU:HD23	1:E:129:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:512:GLN:HG2	2:H:592:GLN:HE22	1.84	0.43
1:E:132:GLU:H	1:E:132:GLU:HG2	1.35	0.43
2:F:612:ASN:O	2:F:616:ILE:HG12	2.19	0.43
1:E:62:ALA:HB3	1:E:69:ILE:HB	2.01	0.43
1:G:205:ASP:HB3	1:G:227:GLN:HB3	2.00	0.43
2:B:709:LEU:O	2:B:713:THR:HG23	2.18	0.43
2:D:622:LEU:HD12	2:D:634:LEU:HD12	2.01	0.43
2:H:616:ILE:HD12	2:H:643:LYS:HG3	2.01	0.43
2:H:593:TRP:HA	2:H:596:ILE:HD12	2.01	0.42
1:C:12:ILE:HG13	2:D:400:LYS:HA	2.01	0.42
2:F:709:LEU:O	2:F:713:THR:HG23	2.19	0.42
1:G:212:TRP:CE3	1:G:222:LEU:HD21	2.54	0.42
2:B:663:ASN:C	1:C:285:LEU:HD21	2.39	0.42
2:D:384:ALA:HA	2:D:393:VAL:O	2.20	0.42
1:E:95:HIS:CE1	1:E:128:VAL:CG2	3.00	0.42
1:E:155:PRO:HD3	1:E:212:TRP:CD1	2.53	0.42
2:B:604:TYR:HB3	2:B:607:ASP:HB3	2.02	0.42
2:F:571:ARG:HG2	2:F:584:LEU:HD12	2.02	0.42
1:E:74:SER:OG	1:E:75:TYR:N	2.53	0.42
1:A:180:ASN:N	1:A:180:ASN:HD22	2.17	0.42
1:A:226:SER:HB3	1:A:228:ASP:OD1	2.20	0.42
1:G:208:ARG:HH22	2:H:376:TRP:HA	1.85	0.42
1:A:11:LEU:O	1:A:28:SER:HB2	2.20	0.42
1:C:239:GLU:O	1:C:240:GLN:HG2	2.20	0.42
2:B:381:SER:HA	2:B:382:PRO:HD3	1.95	0.42
1:C:132:GLU:H	1:C:132:GLU:HG2	1.48	0.42
2:H:622:LEU:HD12	2:H:634:LEU:CD1	2.49	0.42
1:A:73:CYS:HB2	1:A:102:VAL:HG12	2.01	0.42
2:B:546:SER:HB2	2:B:548:ASN:HD22	1.85	0.42
2:B:535:LEU:HB3	2:B:538:GLU:HG2	2.02	0.41
2:B:737:LYS:O	2:B:741:LEU:HB2	2.20	0.41
2:D:551:LEU:O	2:D:555:VAL:HG23	2.19	0.41
2:H:649:LEU:HD13	2:H:698:GLN:HB3	2.01	0.41
2:D:604:TYR:CZ	2:D:610:GLN:HG2	2.54	0.41
1:C:215:THR:HG23	1:C:217:LEU:H	1.85	0.41
2:F:384:ALA:HA	2:F:393:VAL:O	2.20	0.41
2:F:386:TRP:HH2	2:F:409:ILE:HD11	1.86	0.41
1:G:74:SER:HB3	1:G:76:ASP:OD1	2.21	0.41
2:H:716:PHE:HD2	2:H:740:VAL:HG13	1.86	0.41
1:A:37:GLU:HG3	1:A:46:ILE:HD11	2.01	0.41
1:A:132:GLU:H	1:A:132:GLU:HG2	1.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:HB2	1:A:288:LYS:HD3	2.01	0.41
2:F:595:PHE:CE1	2:H:516:LYS:HG2	2.56	0.41
2:D:696:ASN:O	2:D:700:ILE:HG12	2.20	0.41
1:E:180:ASN:N	1:E:180:ASN:ND2	2.69	0.41
2:F:549:GLU:O	2:F:550:ARG:HB2	2.20	0.41
1:C:181:LEU:CD2	1:C:201:GLU:HG2	2.51	0.41
2:D:527:VAL:O	2:D:531:LEU:HG	2.21	0.41
1:E:213:SER:HA	1:E:214:PRO:HD3	1.89	0.41
2:F:643:LYS:O	2:F:647:ILE:HG12	2.21	0.41
1:G:179:ASP:O	1:G:180:ASN:HB2	2.21	0.41
1:G:222:LEU:O	1:G:233:ILE:HA	2.21	0.41
2:B:604:TYR:CZ	2:B:610:GLN:HG2	2.55	0.41
1:C:74:SER:OG	1:C:75:TYR:N	2.53	0.40
2:F:681:PHE:O	2:F:685:SER:HB2	2.21	0.40
2:F:549:GLU:HG3	2:F:550:ARG:H	1.86	0.40
2:F:696:ASN:O	2:F:700:ILE:HG12	2.22	0.40
2:F:703:PHE:O	2:F:707:ILE:HG12	2.22	0.40
2:H:702:LYS:HD3	2:H:702:LYS:HA	1.84	0.40
1:A:179:ASP:O	1:A:180:ASN:HB2	2.21	0.40
1:E:131:LYS:HB2	1:E:135:THR:O	2.22	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	275/297 (93%)	259 (94%)	14 (5%)	2 (1%)	22	53
1	C	275/297 (93%)	259 (94%)	15 (6%)	1 (0%)	34	66
1	E	275/297 (93%)	258 (94%)	13 (5%)	4 (2%)	10	33
1	G	275/297 (93%)	260 (94%)	13 (5%)	2 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	323/345 (94%)	304 (94%)	15 (5%)	4 (1%)	13 39
2	D	323/345 (94%)	300 (93%)	21 (6%)	2 (1%)	25 56
2	F	323/345 (94%)	299 (93%)	22 (7%)	2 (1%)	25 56
2	H	323/345 (94%)	303 (94%)	18 (6%)	2 (1%)	25 56
All	All	2392/2568 (93%)	2242 (94%)	131 (6%)	19 (1%)	19 49

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	ILE
2	D	378	GLY
2	F	380	PRO
2	H	378	GLY
2	H	380	PRO
1	A	146	ILE
2	B	378	GLY
2	B	566	LYS
2	B	607	ASP
2	D	437	LYS
1	E	275	ASP
2	B	564	GLY
1	E	6	ASN
1	A	202	GLY
1	E	51	GLY
1	E	202	GLY
1	G	146	ILE
1	G	202	GLY
2	F	564	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	237/252 (94%)	228 (96%)	9 (4%)	33 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	237/252 (94%)	225 (95%)	12 (5%)	24 55
1	E	237/252 (94%)	227 (96%)	10 (4%)	30 63
1	G	237/252 (94%)	230 (97%)	7 (3%)	41 75
2	B	292/306 (95%)	282 (97%)	10 (3%)	37 71
2	D	292/306 (95%)	282 (97%)	10 (3%)	37 71
2	F	292/306 (95%)	282 (97%)	10 (3%)	37 71
2	H	292/306 (95%)	284 (97%)	8 (3%)	44 78
All	All	2116/2232 (95%)	2040 (96%)	76 (4%)	35 69

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	104	SER
1	A	128	VAL
1	A	132	GLU
1	A	152	SER
1	A	197	GLU
1	A	238	ASN
1	A	247	LEU
1	A	251	GLU
2	B	439	ILE
2	B	458	THR
2	B	509	ASN
2	B	511	GLU
2	B	534	ASP
2	B	538	GLU
2	B	572	ILE
2	B	606	ASN
2	B	641	LEU
2	B	695	ASN
1	C	10	GLU
1	C	88	ARG
1	C	132	GLU
1	C	215	THR
1	C	216	VAL
1	C	225	VAL
1	C	238	ASN
1	C	247	LEU
1	C	251	GLU

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Mol	Chain	Res	Type
1	C	265	SER
1	C	271	LEU
1	C	276	ASN
2	D	439	ILE
2	D	458	THR
2	D	511	GLU
2	D	537	MET
2	D	538	GLU
2	D	582	ASP
2	D	606	ASN
2	D	642	ASP
2	D	695	ASN
2	D	721	GLU
1	E	88	ARG
1	E	132	GLU
1	E	157	THR
1	E	225	VAL
1	E	238	ASN
1	E	240	GLN
1	E	247	LEU
1	E	251	GLU
1	E	271	LEU
1	E	276	ASN
2	F	398	ASP
2	F	417	THR
2	F	439	ILE
2	F	511	GLU
2	F	537	MET
2	F	538	GLU
2	F	572	ILE
2	F	606	ASN
2	F	630	ASP
2	F	695	ASN
1	G	50	THR
1	G	88	ARG
1	G	132	GLU
1	G	225	VAL
1	G	240	GLN
1	G	247	LEU
1	G	265	SER
2	H	439	ILE
2	H	458	THR

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Mol	Chain	Res	Type
2	H	534	ASP
2	H	590	VAL
2	H	606	ASN
2	H	689	ASN
2	H	695	ASN
2	H	721	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	149	ASN
1	A	180	ASN
2	B	517	ASN
2	B	548	ASN
2	B	695	ASN
1	C	149	ASN
1	C	180	ASN
2	D	695	ASN
1	E	110	HIS
1	E	149	ASN
1	E	180	ASN
2	F	385	HIS
2	F	448	ASN
2	F	509	ASN
2	F	517	ASN
2	F	625	ASN
2	F	695	ASN
2	F	698	GLN
1	G	110	HIS
1	G	149	ASN
1	G	180	ASN
1	G	276	ASN
2	H	448	ASN
2	H	509	ASN
2	H	592	GLN
2	H	602	ASN
2	H	695	ASN

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 monosaccharides 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	279/297 (93%)	-0.05	1 (0%)	92	91	25, 39, 59, 73	0
1	C	279/297 (93%)	0.01	1 (0%)	92	91	25, 38, 58, 73	0
1	E	279/297 (93%)	-0.04	3 (1%)	80	75	25, 38, 59, 73	0
1	G	279/297 (93%)	-0.08	1 (0%)	92	91	25, 38, 58, 73	0
2	B	329/345 (95%)	0.50	20 (6%)	21	13	34, 59, 80, 98	0
2	D	329/345 (95%)	0.32	9 (2%)	54	44	34, 59, 80, 98	0
2	F	329/345 (95%)	0.36	8 (2%)	59	49	34, 59, 80, 98	0
2	H	329/345 (95%)	0.41	14 (4%)	35	25	34, 59, 80, 98	0
All	All	2432/2568 (94%)	0.20	57 (2%)	60	51	25, 51, 74, 98	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	730	ASN	6.2
2	B	745	GLY	5.4
2	B	729	ASP	5.1
2	B	731	GLU	4.8
2	B	376	TRP	4.8
2	H	508	GLY	4.2
2	D	547	ASN	4.0
2	H	449	LEU	4.0
2	B	378	GLY	3.9
2	D	376	TRP	3.8
2	H	468	PHE	3.8
2	D	735	THR	3.7
2	F	439	ILE	3.6
2	D	548	ASN	3.5
2	B	469	ASP	3.5
2	F	376	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	696	ASN	3.3
2	B	728	SER	3.2
1	A	240	GLN	3.2
2	B	431	ILE	3.1
2	B	458	THR	3.1
2	H	512	GLN	3.1
1	E	215	THR	3.1
2	B	377	TYR	3.0
2	D	546	SER	3.0
1	G	135	THR	2.9
2	B	564	GLY	2.9
2	F	380	PRO	2.9
2	H	467	ALA	2.8
2	H	731	GLU	2.8
2	D	452	LYS	2.7
2	D	689	ASN	2.7
2	D	551	LEU	2.7
2	H	376	TRP	2.6
2	B	694	ILE	2.6
1	E	216	VAL	2.6
2	D	732	GLU	2.5
2	B	711	THR	2.5
2	F	547	ASN	2.5
2	F	653	PRO	2.5
2	B	425	LYS	2.5
2	F	377	TYR	2.4
2	B	463	LYS	2.4
2	F	580	GLU	2.3
2	H	737	LYS	2.3
2	H	734	LYS	2.3
2	H	730	ASN	2.2
2	B	736	GLU	2.2
2	H	377	TYR	2.2
2	H	616	ILE	2.1
2	B	422	LEU	2.1
2	H	431	ILE	2.1
2	B	441	ASP	2.1
1	C	239	GLU	2.1
2	H	559	TYR	2.1
1	E	276	ASN	2.0
2	F	548	ASN	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.