Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:50 am BST

PDB ID	:	6IW5
Title	:	Crystal structure of YFV-China sE in prefusion state
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Deposited on	:	2018-12-04
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

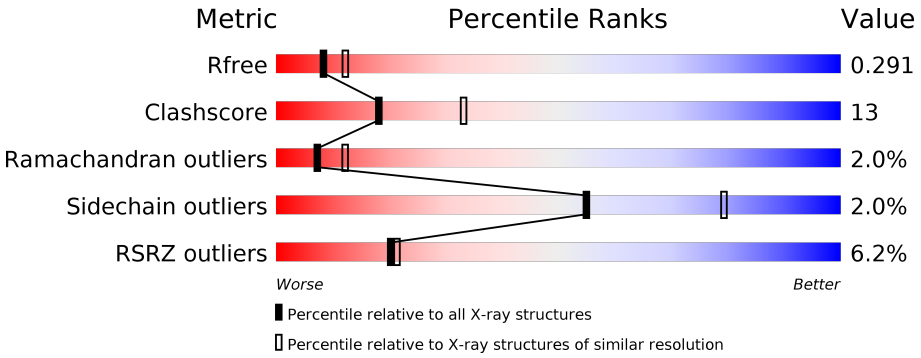
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	393	3% 77% 23%
1	B	393	8% 68% 29% .
1	C	393	8% 70% 27% ..
1	D	393	5% 71% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12133 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 Envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			2995	1875	517	583	20			
1	B	393	Total	C	N	O	S	0	0	0
			2995	1875	517	583	20			
1	C	393	Total	C	N	O	S	0	0	0
			2995	1875	517	583	20			
1	D	393	Total	C	N	O	S	0	0	0
			2995	1875	517	583	20			

- Molecule 2 is water.

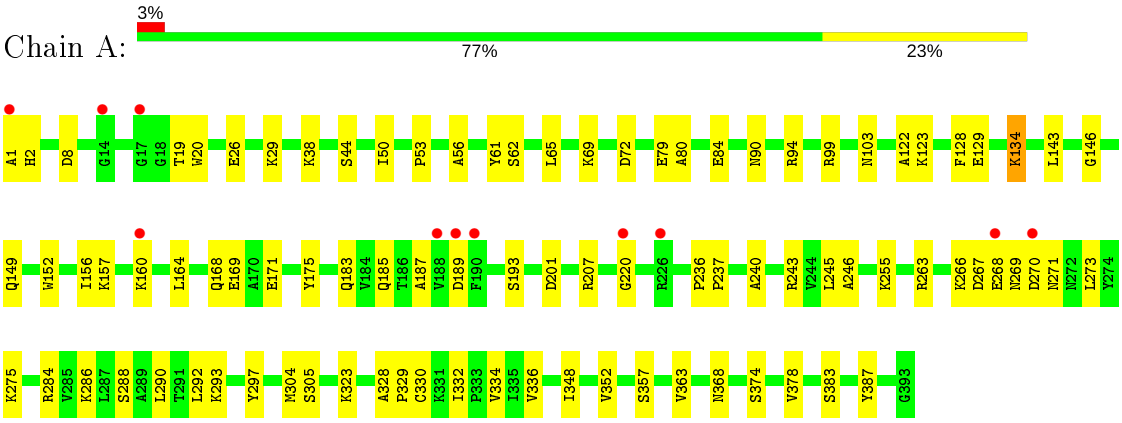
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	47	Total	O	0	0
			47	47		
2	C	34	Total	O	0	0
			34	34		
2	D	32	Total	O	0	0
			32	32		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

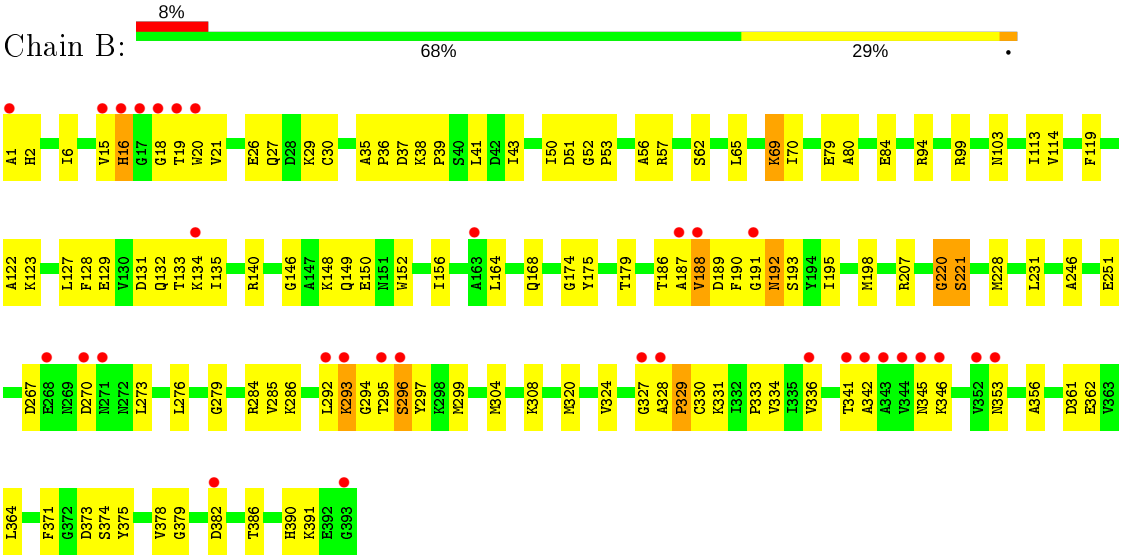
- Molecule 1: Envelope protein

Chain A:



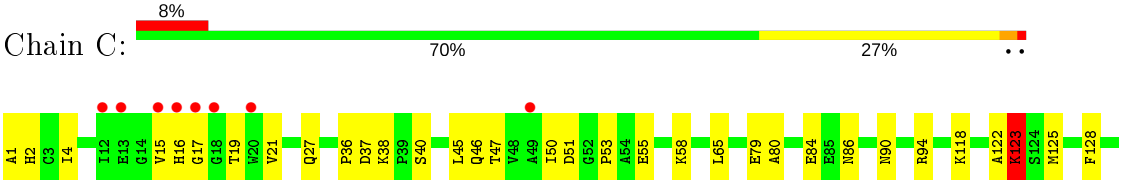
- Molecule 1: Envelope protein

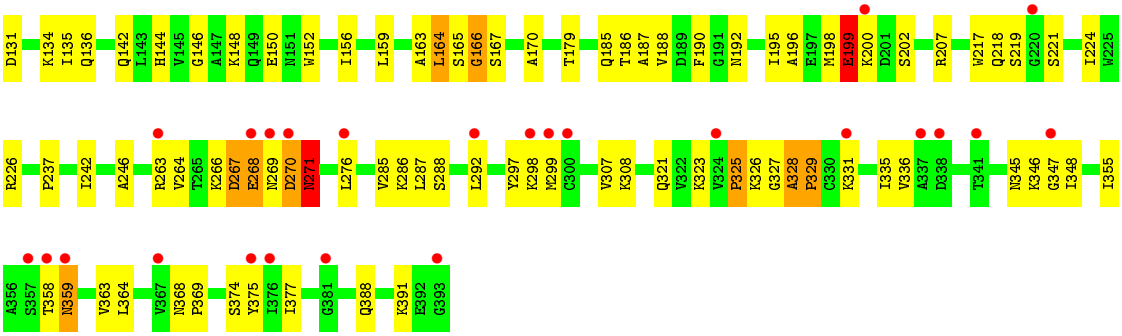
Chain B:



- Molecule 1: Envelope protein

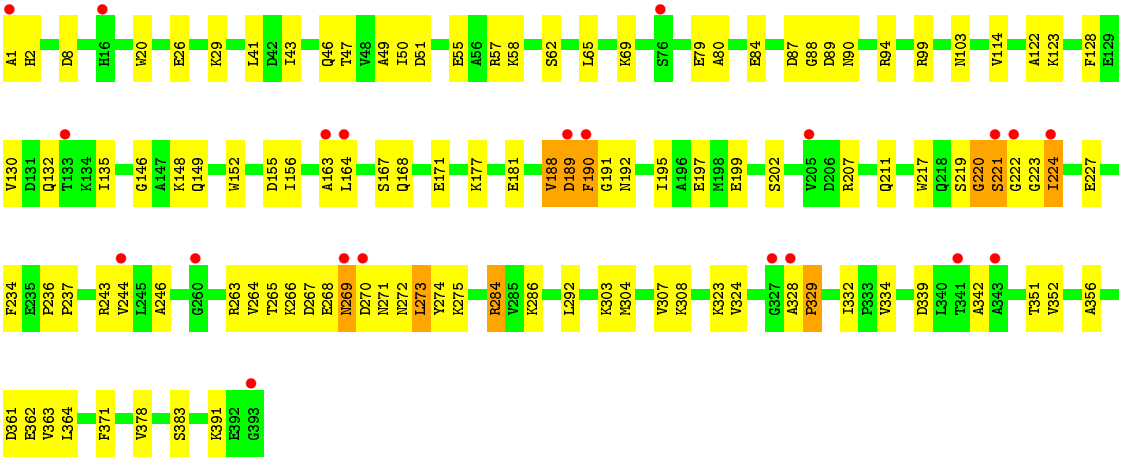
Chain C:





- Molecule 1: Envelope protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.78Å 121.36Å 101.58Å 90.00° 93.46° 90.00°	Depositor
Resolution (Å)	46.78 – 2.50 49.08 – 2.49	Depositor EDS
% Data completeness (in resolution range)	78.7 (46.78-2.50) 78.7 (49.08-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.236 , 0.292 0.239 , 0.291	Depositor DCC
R_{free} test set	2202 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12133	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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

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	0.30	0/3055	0.63	1/4145 (0.0%)
1	B	0.34	0/3055	0.66	2/4145 (0.0%)
1	C	0.34	0/3055	0.70	3/4145 (0.1%)
1	D	0.32	0/3055	0.63	1/4145 (0.0%)
All	All	0.32	0/12220	0.66	7/16580 (0.0%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	270	ASP	C-N-CA	7.15	139.57	121.70
1	D	273	LEU	CB-CG-CD1	-6.38	100.15	111.00
1	B	273	LEU	CA-CB-CG	6.16	129.46	115.30
1	A	270	ASP	N-CA-C	-5.95	94.93	111.00
1	C	123	LYS	CD-CE-NZ	-5.31	99.48	111.70
1	B	168	GLN	CA-CB-CG	5.26	124.97	113.40
1	C	267	ASP	CB-CG-OD2	-5.09	113.72	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	293	LYS	Peptide

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	2995	0	2934	54	0
1	B	2995	0	2934	95	0
1	C	2995	0	2934	86	1
1	D	2995	0	2934	84	1
2	A	40	0	0	9	0
2	B	47	0	0	11	1
2	C	34	0	0	8	1
2	D	32	0	0	4	0
All	All	12133	0	11736	317	2

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 13.

All (317) 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:C:308:LYS:HD2	1:C:321:GLN:HE21	1.20	1.01
1:A:65:LEU:O	2:A:401:HOH:O	1.83	0.95
1:B:304:MET:SD	2:B:446:HOH:O	2.24	0.93
1:B:27:GLN:OE1	2:B:401:HOH:O	1.88	0.89
1:A:80:ALA:O	1:A:94:ARG:NH2	2.07	0.88
1:A:297:TYR:O	2:A:402:HOH:O	1.92	0.87
1:B:132:GLN:OE1	2:B:402:HOH:O	1.95	0.84
1:B:336:VAL:N	1:B:345:ASN:OD1	2.12	0.82
1:D:308:LYS:NZ	2:D:402:HOH:O	2.13	0.82
1:B:276:LEU:O	2:B:403:HOH:O	1.97	0.81
1:C:308:LYS:HD2	1:C:321:GLN:NE2	1.94	0.81
1:D:122:ALA:O	1:D:123:LYS:HD3	1.82	0.80
1:B:362:GLU:OE2	2:B:404:HOH:O	2.01	0.79
1:C:308:LYS:HB2	1:C:321:GLN:HB3	1.65	0.79
1:C:16:HIS:CD2	1:C:36:PRO:HG3	2.18	0.79
1:B:135:ILE:HD11	1:B:190:PHE:HZ	1.49	0.77
1:D:351:THR:OG1	2:D:401:HOH:O	1.97	0.76
1:B:51:ASP:O	1:B:134:LYS:HE3	1.86	0.76
1:B:70:ILE:HD11	1:B:113:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:O	1:C:94:ARG:NH2	2.19	0.75
1:B:135:ILE:HD11	1:B:190:PHE:CZ	2.22	0.74
1:D:269:ASN:H	1:D:269:ASN:HD22	1.37	0.73
1:D:271:ASN:O	1:D:273:LEU:HB2	1.89	0.73
1:C:131:ASP:HB3	1:C:134:LYS:HD2	1.69	0.73
1:B:324:VAL:HG12	1:B:327:GLY:HA3	1.71	0.73
1:A:157:LYS:NZ	1:A:171:GLU:O	2.23	0.72
1:B:346:LYS:O	1:B:346:LYS:HG3	1.89	0.72
1:B:293:LYS:HG3	1:B:294:GLY:H	1.55	0.72
1:D:269:ASN:N	1:D:269:ASN:HD22	1.89	0.71
1:C:45:LEU:O	2:C:401:HOH:O	2.08	0.71
1:C:94:ARG:NH1	2:C:405:HOH:O	2.24	0.71
1:B:190:PHE:O	1:B:192:ASN:N	2.23	0.70
1:A:255:LYS:O	2:A:403:HOH:O	2.08	0.70
1:A:348:ILE:HG23	1:A:368:ASN:HB3	1.74	0.69
1:A:357:SER:HB3	1:B:270:ASP:HB3	1.74	0.69
1:B:293:LYS:HD2	1:B:295:THR:H	1.57	0.69
1:B:50:ILE:HG23	1:B:134:LYS:HG2	1.75	0.69
1:B:16:HIS:C	1:B:18:GLY:H	1.96	0.69
1:C:276:LEU:O	2:C:402:HOH:O	2.09	0.69
1:A:84:GLU:HB3	1:A:90:ASN:HD22	1.56	0.69
1:B:320:MET:HE1	1:B:378:VAL:HG21	1.73	0.69
1:C:355:ILE:HG13	2:C:415:HOH:O	1.92	0.68
1:B:53:PRO:HA	1:B:134:LYS:HZ3	1.58	0.68
1:B:16:HIS:NE2	1:B:35:ALA:HB1	2.09	0.67
1:D:89:ASP:OD1	1:D:90:ASN:ND2	2.27	0.67
1:B:29:LYS:NZ	2:B:409:HOH:O	2.26	0.67
1:A:268:GLU:HG2	1:A:269:ASN:N	2.10	0.66
1:C:150:GLU:OE1	2:C:403:HOH:O	2.12	0.66
1:D:220:GLY:O	1:D:222:GLY:N	2.27	0.66
1:D:270:ASP:O	1:D:271:ASN:HB3	1.96	0.66
1:A:383:SER:OG	2:A:404:HOH:O	2.12	0.66
1:D:26:GLU:HB2	1:D:29:LYS:HD2	1.78	0.65
1:A:56:ALA:HB2	1:A:129:GLU:HG3	1.79	0.65
1:D:181:GLU:OE1	1:D:284:ARG:NH1	2.28	0.64
1:A:267:ASP:OD1	1:A:268:GLU:N	2.28	0.64
1:D:79:GLU:HG3	1:D:94:ARG:HH22	1.62	0.64
1:A:169:GLU:OE1	2:A:405:HOH:O	2.15	0.64
1:D:223:GLY:O	1:D:224:ILE:HG13	1.99	0.63
1:B:26:GLU:HB2	1:B:29:LYS:HD2	1.81	0.63
1:D:65:LEU:HG	1:D:246:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASP:OD1	1:B:390:HIS:ND1	2.31	0.62
1:C:269:ASN:N	2:C:408:HOH:O	2.31	0.62
1:D:217:TRP:NE1	1:D:227:GLU:OE1	2.32	0.62
1:A:26:GLU:HB2	1:A:29:LYS:HD3	1.82	0.62
1:B:328:ALA:HB1	1:B:329:PRO:HD2	1.81	0.62
1:C:271:ASN:HA	2:C:408:HOH:O	2.00	0.61
1:C:27:GLN:NE2	2:C:402:HOH:O	2.25	0.61
1:C:122:ALA:O	1:C:123:LYS:HD3	2.00	0.61
1:B:190:PHE:C	1:B:192:ASN:H	2.02	0.61
1:A:38:LYS:NZ	1:A:290:LEU:O	2.29	0.60
1:D:99:ARG:NH2	1:D:103:ASN:O	2.33	0.60
1:B:333:PRO:HG2	1:B:379:GLY:HA2	1.83	0.60
1:B:53:PRO:HA	1:B:134:LYS:NZ	2.16	0.60
1:B:361:ASP:OD1	1:B:362:GLU:N	2.34	0.60
1:B:220:GLY:HA3	1:B:221:SER:CB	2.31	0.60
1:C:186:THR:O	1:C:188:VAL:N	2.35	0.60
1:D:69:LYS:NZ	1:D:84:GLU:HG2	2.17	0.59
1:C:299:MET:HG3	1:C:331:LYS:HE2	1.83	0.59
1:A:266:LYS:HA	1:A:273:LEU:O	2.02	0.59
1:C:1:ALA:N	1:C:2:HIS:HA	2.16	0.59
1:D:334:VAL:HG22	1:D:378:VAL:HG22	1.83	0.59
1:D:271:ASN:O	1:D:273:LEU:N	2.36	0.58
1:D:269:ASN:N	1:D:269:ASN:ND2	2.52	0.58
1:D:266:LYS:HA	1:D:273:LEU:O	2.04	0.58
1:D:171:GLU:HG3	1:D:177:LYS:HB3	1.86	0.58
1:D:135:ILE:HD11	1:D:190:PHE:CZ	2.39	0.58
1:C:267:ASP:OD2	1:C:270:ASP:HB3	2.04	0.57
1:B:174:GLY:O	1:B:293:LYS:HB2	2.04	0.57
1:D:268:GLU:HB3	1:D:269:ASN:ND2	2.19	0.57
1:C:335:ILE:HG13	1:C:377:ILE:HB	1.87	0.57
1:B:293:LYS:HA	1:B:295:THR:HG23	1.85	0.56
1:C:179:THR:HB	1:C:286:LYS:HB3	1.87	0.56
1:A:19:THR:HG23	1:A:288:SER:HB3	1.87	0.56
1:C:299:MET:CG	1:C:331:LYS:HE2	2.35	0.56
1:D:307:VAL:HG23	1:D:323:LYS:HB2	1.87	0.56
1:A:304:MET:HE3	1:A:332:ILE:HG12	1.88	0.56
1:B:267:ASP:OD2	1:B:267:ASP:N	2.39	0.56
1:D:49:ALA:HB1	1:D:273:LEU:HG	1.88	0.55
1:B:37:ASP:OD2	2:B:406:HOH:O	2.18	0.55
1:C:307:VAL:HG23	1:C:323:LYS:HB2	1.87	0.55
1:B:56:ALA:HB2	1:B:129:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG22	1:C:345:ASN:HB2	1.88	0.55
1:A:44:SER:HA	2:A:418:HOH:O	2.06	0.55
1:C:21:VAL:HG23	1:C:285:VAL:HB	1.88	0.55
1:D:123:LYS:HE3	1:D:199:GLU:OE2	2.07	0.55
1:C:217:TRP:O	1:C:226:ARG:HG3	2.07	0.55
1:D:202:SER:HB2	1:D:264:VAL:O	2.07	0.55
1:B:175:TYR:CZ	1:B:293:LYS:HB3	2.42	0.54
1:D:303:LYS:HB2	1:D:383:SER:HB2	1.88	0.54
1:D:324:VAL:HG21	1:D:356:ALA:HB2	1.90	0.54
1:C:131:ASP:HB3	1:C:134:LYS:HB2	1.89	0.54
1:D:263:ARG:NH2	2:D:405:HOH:O	2.34	0.54
1:A:160:LYS:O	1:A:168:GLN:NE2	2.41	0.54
1:A:328:ALA:O	1:A:330:CYS:N	2.42	0.53
1:B:324:VAL:CG1	1:B:327:GLY:HA3	2.37	0.53
1:A:201:ASP:HB3	1:A:263:ARG:HH12	1.73	0.53
1:D:265:THR:O	1:D:275:LYS:HE2	2.07	0.53
1:D:1:ALA:N	1:D:2:HIS:HA	2.24	0.53
1:C:46:GLN:HG2	1:C:47:THR:HG23	1.90	0.53
1:B:50:ILE:CG2	1:B:134:LYS:HG2	2.39	0.53
1:A:65:LEU:HG	1:A:246:ALA:HB2	1.91	0.53
1:C:16:HIS:CG	1:C:36:PRO:HG3	2.44	0.53
1:D:149:GLN:HA	1:D:152:TRP:CE2	2.44	0.53
1:D:292:LEU:HD21	1:D:352:VAL:HG12	1.91	0.53
1:B:51:ASP:C	1:B:134:LYS:HE3	2.29	0.52
1:D:1:ALA:H3	1:D:2:HIS:HA	1.74	0.52
1:C:123:LYS:NZ	1:C:199:GLU:OE1	2.42	0.52
1:D:243:ARG:HH11	1:D:243:ARG:HG3	1.73	0.52
1:D:268:GLU:HB3	1:D:269:ASN:HD22	1.73	0.52
1:B:299:MET:HA	1:B:331:LYS:H	1.75	0.52
1:A:62:SER:HB3	1:A:123:LYS:HB2	1.92	0.51
1:B:16:HIS:CD2	1:B:35:ALA:HB1	2.45	0.51
1:B:330:CYS:SG	1:B:331:LYS:N	2.83	0.51
1:C:186:THR:O	1:C:188:VAL:HG12	2.11	0.51
1:D:304:MET:HE3	1:D:332:ILE:HG12	1.93	0.51
1:C:65:LEU:HG	1:C:246:ALA:HB2	1.92	0.51
1:B:149:GLN:HA	1:B:152:TRP:CE2	2.46	0.51
1:C:298:LYS:O	1:C:331:LYS:N	2.42	0.51
1:B:16:HIS:C	1:B:18:GLY:N	2.64	0.51
1:A:175:TYR:CE1	1:A:293:LYS:HD3	2.46	0.51
1:C:90:ASN:ND2	1:C:118:LYS:HA	2.26	0.50
1:C:297:TYR:O	1:C:331:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLY:O	1:C:359:ASN:ND2	2.44	0.50
1:C:128:PHE:HB2	1:C:195:ILE:HB	1.94	0.50
1:B:293:LYS:CG	1:B:294:GLY:H	2.22	0.50
1:C:2:HIS:HE1	1:C:4:ILE:HD12	1.77	0.50
1:A:8:ASP:HB3	1:A:29:LYS:HG2	1.95	0.49
1:B:220:GLY:HA3	1:B:221:SER:HB3	1.95	0.49
1:C:38:LYS:HE3	1:C:287:LEU:O	2.12	0.49
1:C:325:PRO:O	1:C:326:LYS:HD3	2.12	0.49
1:D:55:GLU:OE1	1:D:58:LYS:HE3	2.12	0.49
1:C:146:GLY:HA2	1:C:364:LEU:O	2.12	0.49
1:C:1:ALA:N	1:C:142:GLN:HB3	2.28	0.49
1:C:152:TRP:O	1:C:156:ILE:HG13	2.12	0.49
1:B:128:PHE:HB2	1:B:195:ILE:HB	1.95	0.49
1:B:378:VAL:HG12	2:B:446:HOH:O	2.12	0.49
1:A:334:VAL:HG22	1:A:378:VAL:HG22	1.94	0.48
1:D:243:ARG:HG3	1:D:243:ARG:NH1	2.27	0.48
1:C:192:ASN:C	1:C:207:ARG:HG3	2.33	0.48
1:C:327:GLY:C	1:C:359:ASN:ND2	2.67	0.48
1:C:369:PRO:HG2	1:C:391:LYS:HD2	1.94	0.48
1:C:79:GLU:HG3	1:C:94:ARG:HH22	1.77	0.48
1:B:21:VAL:HG23	1:B:285:VAL:HB	1.96	0.48
1:A:20:TRP:CH2	1:A:286:LYS:HB2	2.49	0.48
1:D:267:ASP:CG	1:D:268:GLU:H	2.17	0.48
1:D:69:LYS:HZ1	1:D:84:GLU:HG2	1.78	0.48
1:B:16:HIS:HE1	1:B:38:LYS:HE3	1.79	0.48
1:C:267:ASP:OD1	1:C:268:GLU:N	2.47	0.48
1:C:199:GLU:HB3	1:C:200:LYS:HD2	1.95	0.48
1:B:80:ALA:O	1:B:94:ARG:NH1	2.41	0.48
1:C:159:LEU:HD11	1:C:170:ALA:HB2	1.96	0.48
1:C:202:SER:HB2	1:C:264:VAL:O	2.14	0.48
1:A:62:SER:O	1:A:122:ALA:N	2.47	0.47
1:B:52:GLY:C	1:B:134:LYS:HZ1	2.15	0.47
1:B:80:ALA:HB3	1:B:114:VAL:HG23	1.95	0.47
1:C:51:ASP:HB2	1:C:136:GLN:HE22	1.78	0.47
1:B:334:VAL:HG22	1:B:378:VAL:HG22	1.95	0.47
1:D:307:VAL:CG2	1:D:323:LYS:HB2	2.43	0.47
1:A:336:VAL:HG12	1:A:374:SER:HB2	1.96	0.47
1:D:328:ALA:HB1	1:D:329:PRO:HD2	1.95	0.47
1:C:348:ILE:HG23	1:C:368:ASN:HB3	1.96	0.47
1:C:135:ILE:HD11	1:C:190:PHE:CZ	2.50	0.47
1:D:128:PHE:HE2	1:D:197:GLU:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:O	2:B:407:HOH:O	2.20	0.47
1:B:53:PRO:HB2	1:B:128:PHE:HB3	1.97	0.47
1:D:57:ARG:HG2	1:D:58:LYS:N	2.30	0.47
1:D:224:ILE:O	1:D:224:ILE:HG22	2.15	0.47
1:B:330:CYS:HB3	1:B:356:ALA:HB3	1.97	0.46
1:C:123:LYS:HD3	1:C:123:LYS:HA	1.64	0.46
1:A:183:GLN:NE2	1:A:185:GLN:OE1	2.49	0.46
1:D:192:ASN:C	1:D:207:ARG:HG3	2.36	0.46
1:C:328:ALA:HB1	1:C:329:PRO:HD2	1.97	0.46
1:D:132:GLN:HG3	1:D:190:PHE:CE2	2.51	0.46
1:D:219:SER:O	1:D:221:SER:N	2.48	0.46
1:D:8:ASP:HB3	1:D:29:LYS:HG2	1.97	0.46
1:A:267:ASP:HB2	1:A:275:LYS:HE2	1.97	0.46
1:A:292:LEU:HD21	1:A:352:VAL:HG12	1.96	0.46
1:B:131:ASP:OD2	1:B:133:THR:OG1	2.33	0.46
1:B:16:HIS:CE1	1:B:38:LYS:HE3	2.51	0.46
1:B:99:ARG:NH2	1:B:103:ASN:O	2.49	0.46
1:B:374:SER:OG	1:B:375:TYR:N	2.47	0.46
1:B:341:THR:OG1	1:B:342:ALA:N	2.49	0.45
1:B:308:LYS:NZ	2:B:405:HOH:O	2.17	0.45
1:B:65:LEU:HG	1:B:246:ALA:HB2	1.99	0.45
1:D:57:ARG:NH1	1:D:211:GLN:HG2	2.32	0.45
1:A:243:ARG:HH21	1:A:245:LEU:HD11	1.81	0.45
1:C:374:SER:O	1:C:388:GLN:HG3	2.16	0.45
1:D:223:GLY:C	1:D:224:ILE:HG13	2.36	0.45
1:A:149:GLN:HA	1:A:152:TRP:CE2	2.52	0.45
1:C:345:ASN:OD1	1:C:347:GLY:N	2.26	0.45
1:A:50:ILE:HG22	1:A:134:LYS:HE2	1.98	0.45
1:D:57:ARG:HH12	1:D:211:GLN:HG2	1.81	0.45
1:B:16:HIS:CD2	2:B:410:HOH:O	2.69	0.45
1:B:119:PHE:HB3	1:B:228:MET:HE3	1.99	0.45
1:A:61:TYR:CZ	1:A:123:LYS:HB3	2.51	0.45
1:C:55:GLU:OE1	1:C:58:LYS:HE2	2.17	0.45
1:D:80:ALA:HB3	1:D:114:VAL:HG23	1.98	0.45
1:D:46:GLN:HG3	1:D:47:THR:HG23	1.99	0.45
1:A:1:ALA:HA	1:A:2:HIS:HA	1.66	0.44
1:D:266:LYS:HD2	1:D:274:TYR:CZ	2.52	0.44
1:D:273:LEU:HA	1:D:273:LEU:HD12	1.65	0.44
1:B:179:THR:HB	1:B:286:LYS:HB3	2.00	0.44
1:B:43:ILE:HA	1:B:140:ARG:O	2.17	0.44
1:C:148:LYS:HE3	1:C:148:LYS:HB2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:MET:HB2	1:C:198:MET:HG2	1.99	0.44
1:C:325:PRO:C	1:C:359:ASN:OD1	2.56	0.44
1:B:16:HIS:CE1	1:B:36:PRO:O	2.71	0.44
1:C:15:VAL:C	1:C:17:GLY:N	2.69	0.44
1:D:128:PHE:HB2	1:D:195:ILE:HB	1.99	0.44
1:D:132:GLN:HG3	1:D:190:PHE:CD2	2.53	0.44
1:A:152:TRP:O	1:A:156:ILE:HG13	2.18	0.44
1:C:345:ASN:OD1	1:C:346:LYS:N	2.50	0.44
1:A:53:PRO:HB2	1:A:128:PHE:HB3	1.98	0.44
1:D:149:GLN:HA	1:D:152:TRP:CD2	2.52	0.44
1:D:80:ALA:O	1:D:94:ARG:NH2	2.46	0.44
1:A:387:TYR:CE2	1:C:164:LEU:HD23	2.53	0.44
1:C:84:GLU:HB3	1:C:90:ASN:OD1	2.17	0.44
1:D:236:PRO:HA	1:D:237:PRO:HD3	1.79	0.44
1:D:267:ASP:HB2	1:D:275:LYS:NZ	2.33	0.43
1:B:296:SER:O	1:B:297:TYR:HB2	2.17	0.43
1:B:16:HIS:ND1	1:B:36:PRO:O	2.51	0.43
1:C:50:ILE:HG23	1:C:134:LYS:HB3	2.00	0.43
1:A:143:LEU:O	2:A:408:HOH:O	2.21	0.43
1:B:62:SER:HB3	1:B:123:LYS:HB2	1.99	0.43
1:B:186:THR:HG21	1:B:190:PHE:CZ	2.53	0.43
1:C:267:ASP:CG	1:C:268:GLU:H	2.22	0.43
1:D:155:ASP:HB3	2:D:425:HOH:O	2.18	0.43
1:A:268:GLU:HG2	1:A:269:ASN:H	1.79	0.43
1:B:6:ILE:HD12	1:B:30:CYS:HB2	2.01	0.43
1:A:84:GLU:HB3	1:A:90:ASN:ND2	2.31	0.43
1:B:293:LYS:HG3	1:B:294:GLY:N	2.29	0.43
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.83	0.43
1:C:336:VAL:HA	1:C:375:TYR:O	2.19	0.43
1:D:146:GLY:HA2	1:D:364:LEU:O	2.18	0.43
1:B:79:GLU:HG3	1:B:94:ARG:HH22	1.83	0.43
1:C:219:SER:C	1:C:221:SER:H	2.23	0.43
1:D:152:TRP:O	1:D:156:ILE:HG13	2.19	0.43
1:D:371:PHE:HA	1:D:391:LYS:HB3	2.01	0.43
1:B:62:SER:O	1:B:122:ALA:N	2.52	0.42
1:C:15:VAL:HG23	1:C:17:GLY:CA	2.49	0.42
1:D:50:ILE:HD13	1:D:130:VAL:HG23	2.01	0.42
1:B:20:TRP:CE3	1:B:284:ARG:HB3	2.54	0.42
1:A:56:ALA:HB2	1:A:129:GLU:CG	2.46	0.42
1:A:79:GLU:OE1	2:A:406:HOH:O	2.21	0.42
1:B:371:PHE:HA	1:B:391:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:HE2	1:B:69:LYS:HB3	1.49	0.42
1:C:53:PRO:HB2	1:C:128:PHE:HB3	2.01	0.42
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.84	0.42
1:B:146:GLY:HA2	1:B:364:LEU:O	2.20	0.42
1:B:39:PRO:HD3	1:B:292:LEU:HD13	2.01	0.42
1:A:189:ASP:OD1	2:A:407:HOH:O	2.21	0.42
1:A:69:LYS:HD2	1:A:84:GLU:HG2	2.02	0.42
1:C:321:GLN:HA	1:C:363:VAL:O	2.19	0.42
1:D:146:GLY:HA3	1:D:363:VAL:HG13	2.01	0.42
1:D:188:VAL:O	1:D:189:ASP:CG	2.57	0.42
1:D:361:ASP:OD1	1:D:362:GLU:N	2.53	0.42
1:D:41:LEU:HD22	1:D:43:ILE:HG23	2.01	0.42
1:D:51:ASP:HA	1:D:273:LEU:CD1	2.49	0.42
1:C:165:SER:HA	1:C:166:GLY:HA3	1.84	0.42
1:C:1:ALA:H3	1:C:2:HIS:HA	1.81	0.42
1:B:148:LYS:HE2	1:B:150:GLU:OE2	2.19	0.42
1:D:41:LEU:CD2	1:D:43:ILE:HG23	2.50	0.42
1:A:146:GLY:HA3	1:A:363:VAL:HG13	2.01	0.42
1:C:163:ALA:O	1:C:164:LEU:HD22	2.20	0.42
1:C:224:ILE:HA	1:C:224:ILE:HD12	1.95	0.41
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.91	0.41
1:A:305:SER:OG	1:A:323:LYS:HB3	2.20	0.41
1:C:164:LEU:HD13	1:C:164:LEU:HA	1.78	0.41
1:B:41:LEU:CD2	1:B:43:ILE:HG23	2.51	0.41
1:C:299:MET:HG3	1:C:331:LYS:CE	2.50	0.41
1:D:148:LYS:HE3	1:D:362:GLU:OE1	2.21	0.41
1:B:152:TRP:O	1:B:156:ILE:HG13	2.20	0.41
1:B:193:SER:N	1:B:207:ARG:HG3	2.36	0.41
1:C:237:PRO:HB3	1:C:242:ILE:HG12	2.02	0.41
1:D:234:PHE:CD2	1:D:244:VAL:HG22	2.55	0.41
1:B:57:ARG:HG3	1:B:127:LEU:HB2	2.03	0.41
1:C:19:THR:HG23	1:C:288:SER:HB3	2.01	0.41
1:B:69:LYS:NZ	1:B:84:GLU:OE1	2.53	0.41
1:D:163:ALA:O	1:D:164:LEU:HD12	2.20	0.41
1:B:1:ALA:HA	1:B:2:HIS:HA	1.60	0.41
1:C:199:GLU:HB3	1:C:200:LYS:H	1.64	0.41
1:D:69:LYS:HZ2	1:D:84:GLU:HG2	1.84	0.41
1:A:193:SER:N	1:A:207:ARG:HG3	2.35	0.41
1:D:267:ASP:HB3	1:D:270:ASP:CG	2.42	0.41
1:D:62:SER:O	1:D:122:ALA:N	2.54	0.41
1:B:220:GLY:HA3	1:B:221:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:SER:HB2	1:C:144:HIS:HB2	2.03	0.41
1:C:266:LYS:HB3	1:C:267:ASP:H	1.58	0.40
1:B:79:GLU:CG	1:B:94:ARG:HH22	2.34	0.40
1:A:236:PRO:HA	1:A:237:PRO:HD3	1.87	0.40
1:C:125:MET:SD	1:C:196:ALA:HB1	2.61	0.40
1:D:339:ASP:OD1	1:D:342:ALA:HB3	2.21	0.40
1:A:72:ASP:OD1	1:A:240:ALA:HB1	2.22	0.40
1:B:198:MET:CE	1:B:251:GLU:HG3	2.51	0.40
1:B:331:LYS:HE2	1:B:353:ASN:HD21	1.87	0.40
1:B:50:ILE:HD12	1:B:195:ILE:HD11	2.03	0.40
1:D:20:TRP:CZ3	1:D:286:LYS:HB2	2.57	0.40

All (2) 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)
2:B:443:HOH:O	2:C:429:HOH:O[2_547]	2.01	0.19
1:C:298:LYS:NZ	1:D:191:GLY:O[1_654]	2.17	0.03

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	391/393 (100%)	360 (92%)	27 (7%)	4 (1%)	15 28
1	B	391/393 (100%)	361 (92%)	21 (5%)	9 (2%)	6 10
1	C	391/393 (100%)	359 (92%)	22 (6%)	10 (3%)	5 8
1	D	391/393 (100%)	363 (93%)	19 (5%)	9 (2%)	6 10
All	All	1564/1572 (100%)	1443 (92%)	89 (6%)	32 (2%)	7 12

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	PRO
1	B	191	GLY
1	B	296	SER
1	B	329	PRO
1	C	187	ALA
1	C	328	ALA
1	C	329	PRO
1	D	221	SER
1	D	272	ASN
1	D	329	PRO
1	A	220	GLY
1	B	189	ASP
1	B	220	GLY
1	C	86	ASN
1	C	166	GLY
1	C	268	GLU
1	C	271	ASN
1	D	88	GLY
1	D	190	PHE
1	D	220	GLY
1	A	271	ASN
1	B	192	ASN
1	C	167	SER
1	C	199	GLU
1	D	167	SER
1	D	189	ASP
1	A	187	ALA
1	B	188	VAL
1	B	221	SER
1	C	325	PRO
1	B	187	ALA
1	D	224	ILE

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	326/326 (100%)	323 (99%)	3 (1%)	78 92
1	B	326/326 (100%)	318 (98%)	8 (2%)	47 73
1	C	326/326 (100%)	316 (97%)	10 (3%)	40 67
1	D	326/326 (100%)	321 (98%)	5 (2%)	65 85
All	All	1304/1304 (100%)	1278 (98%)	26 (2%)	55 79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LYS
1	A	164	LEU
1	A	284	ARG
1	B	15	VAL
1	B	16	HIS
1	B	19	THR
1	B	69	LYS
1	B	164	LEU
1	B	188	VAL
1	B	382	ASP
1	B	386	THR
1	C	37	ASP
1	C	123	LYS
1	C	164	LEU
1	C	185	GLN
1	C	199	GLU
1	C	218	GLN
1	C	263	ARG
1	C	271	ASN
1	C	358	THR
1	C	359	ASN
1	D	87	ASP
1	D	168	GLN
1	D	188	VAL
1	D	269	ASN
1	D	284	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN

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Mol	Chain	Res	Type
1	A	269	ASN
1	B	229	HIS
1	C	16	HIS
1	C	218	GLN
1	C	271	ASN
1	C	353	ASN
1	D	90	ASN
1	D	269	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 carbohydrates 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	393/393 (100%)	0.17	11 (2%)	53	56	12, 38, 78, 115	0
1	B	393/393 (100%)	0.37	32 (8%)	12	12	15, 34, 90, 185	0
1	C	393/393 (100%)	0.60	33 (8%)	11	11	10, 47, 99, 182	0
1	D	393/393 (100%)	0.36	21 (5%)	26	28	14, 42, 89, 149	0
All	All	1572/1572 (100%)	0.37	97 (6%)	20	21	10, 40, 90, 185	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	GLY	7.9
1	C	359	ASN	6.8
1	D	224	ILE	6.7
1	B	344	VAL	6.3
1	B	16	HIS	6.2
1	C	16	HIS	6.2
1	C	15	VAL	5.9
1	C	18	GLY	5.9
1	B	295	THR	5.5
1	B	270	ASP	5.3
1	D	163	ALA	4.6
1	B	187	ALA	4.6
1	C	337	ALA	4.6
1	D	222	GLY	4.5
1	B	271	ASN	4.4
1	D	343	ALA	4.4
1	D	341	THR	4.4
1	B	293	LYS	4.2
1	C	270	ASP	4.0
1	D	164	LEU	3.9
1	D	1	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	300	CYS	3.8
1	B	352	VAL	3.8
1	B	342	ALA	3.7
1	D	189	ASP	3.7
1	B	327	GLY	3.7
1	A	270	ASP	3.5
1	B	393	GLY	3.5
1	B	19	THR	3.5
1	C	341	THR	3.4
1	D	260	GLY	3.4
1	D	269	ASN	3.4
1	D	16	HIS	3.4
1	A	1	ALA	3.3
1	C	381	GLY	3.2
1	B	188	VAL	3.2
1	D	205	VAL	3.1
1	C	375	TYR	3.1
1	A	160	LYS	3.0
1	C	269	ASN	3.0
1	D	270	ASP	3.0
1	C	49	ALA	3.0
1	C	393	GLY	3.0
1	C	263	ARG	2.9
1	C	220	GLY	2.9
1	D	393	GLY	2.9
1	B	343	ALA	2.8
1	B	18	GLY	2.8
1	D	190	PHE	2.8
1	B	336	VAL	2.8
1	C	268	GLU	2.7
1	C	20	TRP	2.7
1	C	276	LEU	2.6
1	C	347	GLY	2.6
1	B	268	GLU	2.6
1	C	324	VAL	2.6
1	C	13	GLU	2.6
1	A	220	GLY	2.6
1	B	292	LEU	2.6
1	C	376	ILE	2.6
1	A	17	GLY	2.5
1	C	338	ASP	2.5
1	B	163	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	358	THR	2.5
1	B	134	LYS	2.5
1	B	1	ALA	2.5
1	D	327	GLY	2.4
1	C	12	ILE	2.4
1	B	15	VAL	2.4
1	B	17	GLY	2.4
1	B	345	ASN	2.4
1	B	353	ASN	2.4
1	B	341	THR	2.3
1	A	14	GLY	2.3
1	C	299	MET	2.3
1	D	328	ALA	2.3
1	B	346	LYS	2.3
1	A	189	ASP	2.2
1	A	190	PHE	2.2
1	C	292	LEU	2.2
1	A	226	ARG	2.2
1	D	76	SER	2.2
1	C	367	VAL	2.2
1	B	382	ASP	2.2
1	C	298	LYS	2.2
1	D	133	THR	2.2
1	B	20	TRP	2.1
1	B	191	GLY	2.1
1	B	328	ALA	2.1
1	C	357	SER	2.1
1	B	296	SER	2.1
1	D	244	VAL	2.1
1	D	221	SER	2.1
1	A	188	VAL	2.0
1	A	268	GLU	2.0
1	C	200	LYS	2.0
1	C	331	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.