WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 01:04 am GMT

PDB ID : 3CPL
Title : Crystal Structure of H-2Db in complex with a variant M6A of the NP366 peptide from influenza A virus
Authors : Kedzierska, K.; Guillonneau, C.; Hatton, L.A.; Stockwell, D.; Gras, S.; Webby, R.; Rossjohn, J.; Purcell, A.W.; Doherty, P.C.; Turner, S.J.
Deposited on : 2008-03-31
Resolution : 2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		25
Ramachandran outliers		2.8%
Sidechain outliers		11.8%
RSRZ outliers		1.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
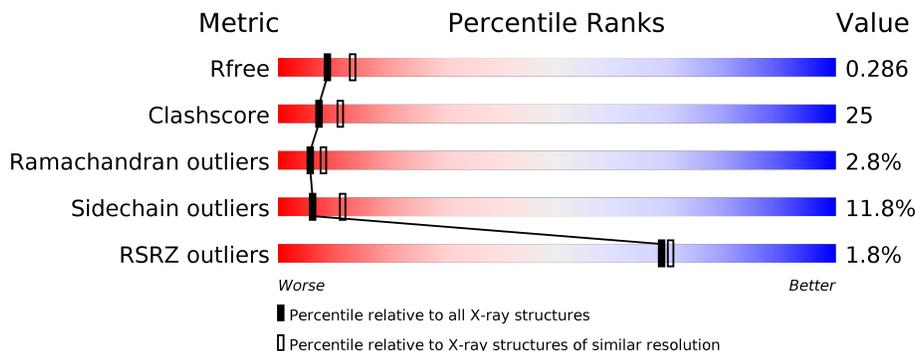
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	275	3% — 53% / 40% / 7%
1	C	275	2% — 55% / 35% / 8% ·
2	B	99	64% / 28% / 7% ·
2	D	99	% — 58% / 38% ·
3	E	9	100%
3	F	9	89% / 11%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6417 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	6	0
			2316	1460	410	437	9			
1	C	275	Total	C	N	O	S	0	3	0
			2285	1440	405	431	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	1	0
			831	530	141	153	7			
2	D	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called NP366 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	S	0	0	0
			66	36	11	18	1			
3	F	9	Total	C	N	O	S	0	0	0
			66	36	11	18	1			

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	4	Total	O	0	0
			4	4		
4	C	10	Total	O	0	0
			10	10		
4	D	10	Total	O	0	0
			10	10		

3 Residue-property plots ⓘ

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: H-2 class I histocompatibility antigen, D-B alpha chain
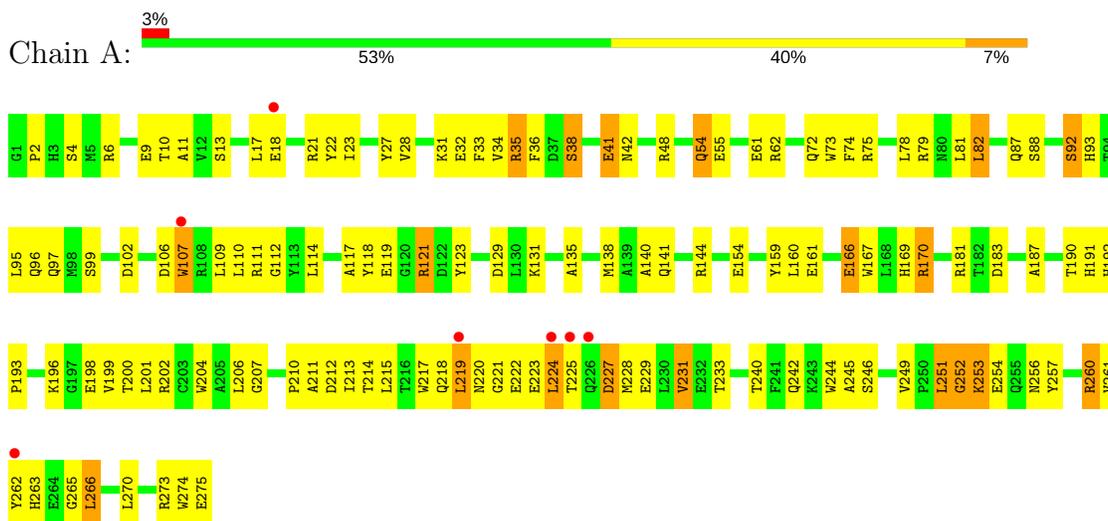
Chain A:

• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain C:

• Molecule 2: Beta-2-microglobulin

Chain B:

I1 Q2 K3 V9 E16 N17 I22 L23 N24 V27 T28 Q29 F30 H31 H34 I37 Q38 M39 L40 K41 N42 K45 K48 V49 D53 M54 S55 W60 S61 F62 Y63 T68 E69 F70 R81 V82 K83 H84 D85 A88 E89 P90 R97 D98 M99

• Molecule 2: Beta-2-microglobulin

Chain D:

%

58% 38% •

I1 Q8 V9 Y10 S11 E16 N17 G18 K19 P20 N21 I22 L23 N24 V27 T28 H31 P32 I37 Q38 M39 L40 K45 I46 P47 K48 V49 E50 D53 K58 D59 W60 Y63 H67 T68 E69 F70 T71 P72 R81 V82 K83 H84 D85 E89 P90 K91

R97 D98 M99

• Molecule 3: NP366 peptide

Chain E:

100%
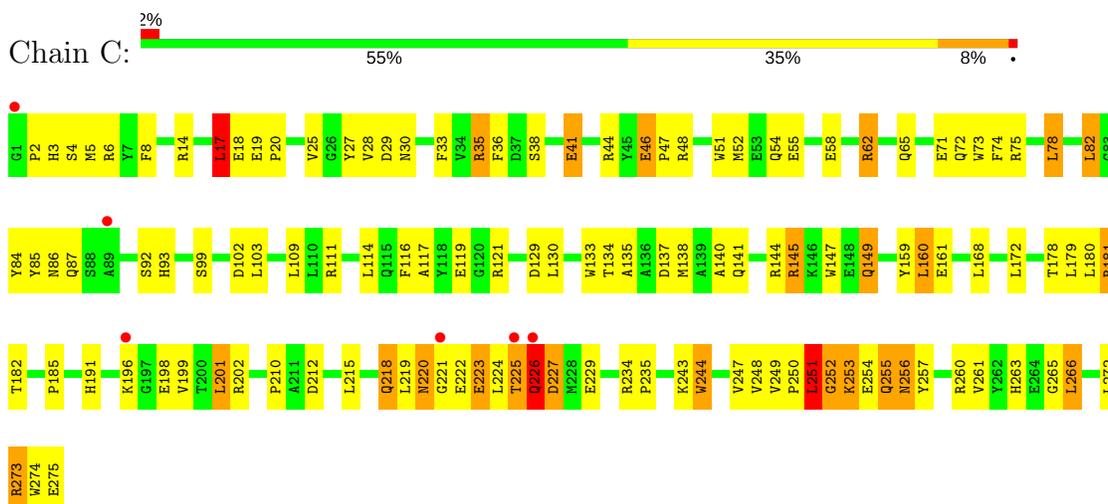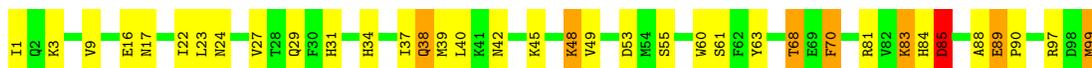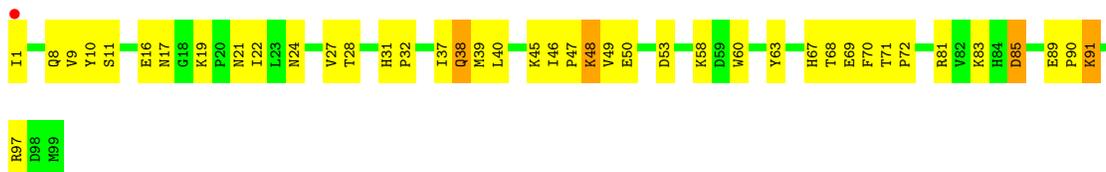
There are no outlier residues recorded for this chain.

• Molecule 3: NP366 peptide

Chain F:

89% 11%

A1 M9
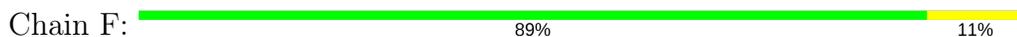
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.71Å 69.70Å 72.38Å 99.95° 111.04° 110.48°	Depositor
Resolution (Å)	15.00 – 2.50 43.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (15.00-2.50) 74.7 (43.88-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.02 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.286 0.221 , 0.286	Depositor DCC
R_{free} test set	3082 reflections (11.23%)	DCC
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 0.0	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.159 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6417	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.56	0/2384	0.68	0/3237
1	C	0.55	0/2351	0.69	1/3191 (0.0%)
2	B	0.59	0/858	0.73	0/1163
2	D	0.57	0/847	0.74	0/1148
3	E	0.78	0/65	0.72	0/85
3	F	0.55	0/65	0.69	0/85
All	All	0.57	0/6570	0.70	1/8909 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	221	GLY	N-CA-C	-5.12	100.31	113.10

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	2316	0	2169	129	0
1	C	2285	0	2149	125	0
2	B	831	0	802	33	0
2	D	821	0	796	42	2
3	E	66	0	57	0	0
3	F	66	0	57	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	0	7	2
4	B	4	0	0	1	0
4	C	10	0	0	7	0
4	D	10	0	0	4	0
All	All	6417	0	6030	310	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 25.

All (310) 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:A:121:ARG:HH11	1:A:121:ARG:CB	1.35	1.40
1:C:201:LEU:CD2	1:C:249:VAL:HG11	1.60	1.29
1:A:121:ARG:NH1	1:A:121:ARG:HB2	1.53	1.21
1:C:168:LEU:HG	1:C:172:LEU:HD11	1.34	1.09
1:C:201:LEU:HD22	1:C:249:VAL:CG1	1.84	1.06
1:A:106[B]:ASP:O	1:A:107[B]:TRP:HB2	1.53	1.03
1:C:181:ARG:HH11	1:C:181:ARG:HG2	0.90	1.03
2:D:39:MET:CE	2:D:49:VAL:HG13	1.88	1.03
1:C:181:ARG:NH1	1:C:181:ARG:HG2	1.68	1.02
1:C:201:LEU:CD2	1:C:249:VAL:CG1	2.37	1.01
1:A:121:ARG:HB2	1:A:121:ARG:HH11	0.81	0.97
1:A:121:ARG:NH1	1:A:121:ARG:CB	2.21	0.94
1:C:201:LEU:HD22	1:C:249:VAL:HG11	1.44	0.94
2:B:17:ASN:HD21	2:B:97:ARG:HH22	1.11	0.94
1:C:134:THR:HA	1:C:144:ARG:HH21	1.32	0.92
1:C:181:ARG:HH11	1:C:181:ARG:CG	1.82	0.91
1:A:106[B]:ASP:O	1:A:107[B]:TRP:CB	2.19	0.90
1:A:260:ARG:NH1	1:A:262:TYR:HD2	1.69	0.90
1:A:260:ARG:HH12	1:A:262:TYR:HD2	1.02	0.90
1:C:219:LEU:O	1:C:220:ASN:O	1.91	0.88
1:C:201:LEU:HD21	1:C:249:VAL:HG11	1.56	0.88
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.54	0.88
1:A:263:HIS:HD2	1:A:265:GLY:H	1.19	0.87
2:D:39:MET:HE3	2:D:49:VAL:HG13	1.54	0.86
1:C:168:LEU:O	1:C:172:LEU:HD12	1.74	0.86
1:A:141:GLN:HE22	1:A:144[A]:ARG:NE	1.73	0.86
1:A:223:GLU:O	1:A:224:LEU:O	1.92	0.85
1:A:141:GLN:HE22	1:A:144[A]:ARG:CD	1.92	0.82
1:C:41:GLU:CD	1:C:41:GLU:H	1.82	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:HIS:CE1	1:C:199:VAL:HG11	2.16	0.81
1:C:133:TRP:NE1	4:C:283:HOH:O	2.12	0.81
1:A:263:HIS:CD2	1:A:265:GLY:H	1.99	0.81
2:D:27:VAL:HG21	2:D:37:ILE:HD13	1.63	0.81
1:C:201:LEU:HD22	1:C:249:VAL:HG12	1.62	0.80
1:C:168:LEU:HG	1:C:172:LEU:CD1	2.08	0.80
1:A:93:HIS:ND1	1:A:119:GLU:OE2	2.11	0.80
1:A:169:HIS:HE1	4:A:281:HOH:O	1.65	0.79
1:A:141:GLN:HE22	1:A:144[A]:ARG:HD3	1.49	0.78
1:C:121:ARG:HB2	1:C:121:ARG:CZ	2.12	0.78
1:C:74:PHE:O	1:C:78:LEU:HB2	1.83	0.78
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.65	0.78
2:D:17:ASN:HD21	2:D:97:ARG:NH2	1.82	0.77
2:D:16:GLU:HA	4:D:106:HOH:O	1.83	0.77
1:A:260:ARG:NH1	1:A:262:TYR:CD2	2.49	0.77
2:D:40:LEU:HD23	2:D:45:LYS:HA	1.66	0.77
1:A:251:LEU:HD23	1:A:252:GLY:H	1.49	0.76
1:C:4:SER:HB3	1:C:102:ASP:OD1	1.84	0.76
1:A:4:SER:HB3	1:A:102:ASP:OD1	1.86	0.75
1:C:14:ARG:HB3	1:C:17:LEU:HD23	1.68	0.75
1:A:229:GLU:HB3	1:A:246:SER:OG	1.86	0.74
1:A:74:PHE:O	1:A:78:LEU:HB2	1.88	0.74
2:B:83:LYS:HE3	2:B:84:HIS:H	1.54	0.73
1:C:62:ARG:HA	1:C:65:GLN:HG2	1.70	0.73
2:B:85:ASP:OD1	2:B:85:ASP:N	2.21	0.73
1:C:253:LYS:N	1:C:253:LYS:HD2	2.02	0.73
1:A:159:TYR:HD2	1:A:160:LEU:HD12	1.53	0.72
1:C:168:LEU:C	1:C:172:LEU:HD12	2.08	0.72
1:A:228:MET:HE2	1:A:245:ALA:HB1	1.71	0.72
1:C:181:ARG:HA	4:C:282:HOH:O	1.90	0.72
2:D:39:MET:HE3	2:D:49:VAL:CG1	2.20	0.71
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.03	0.71
2:D:39:MET:HE2	2:D:49:VAL:HG13	1.72	0.70
1:C:210:PRO:O	1:C:263:HIS:HE1	1.73	0.70
1:A:141:GLN:NE2	1:A:144[A]:ARG:HD3	2.05	0.70
1:A:253:LYS:HD2	1:A:253:LYS:N	2.05	0.70
1:C:103:LEU:HG	1:C:168:LEU:HD23	1.72	0.69
2:D:85:ASP:N	2:D:85:ASP:OD1	2.22	0.69
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.27	0.69
2:D:17:ASN:ND2	2:D:97:ARG:HH22	1.90	0.69
2:B:48:LYS:HG2	4:B:103:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:ASN:HD21	2:D:97:ARG:HH22	1.39	0.69
2:B:39:MET:HE1	2:B:68:THR:HB	1.75	0.68
1:C:251:LEU:HD23	1:C:252:GLY:N	2.07	0.68
2:B:83:LYS:HD2	2:B:90:PRO:HG3	1.75	0.68
1:A:201:LEU:HD21	1:A:249:VAL:HG11	1.75	0.68
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.29	0.68
1:C:62:ARG:HA	1:C:65:GLN:HE21	1.57	0.68
1:C:141:GLN:HE22	1:C:144:ARG:NH1	1.92	0.68
1:C:248:VAL:O	1:C:248:VAL:HG23	1.94	0.67
1:C:253:LYS:HB3	1:C:256:ASN:HD21	1.57	0.67
1:C:179:LEU:C	1:C:181:ARG:H	1.96	0.67
1:A:220:ASN:O	1:A:222:GLU:N	2.28	0.66
1:C:185:PRO:HD2	1:C:266:LEU:CD2	2.26	0.66
1:C:147:TRP:HB3	4:C:283:HOH:O	1.95	0.66
1:C:251:LEU:HD23	1:C:252:GLY:H	1.59	0.66
1:A:13:SER:HB2	1:A:93:HIS:H	1.60	0.65
2:B:17:ASN:HD21	2:B:97:ARG:NH2	1.89	0.65
2:B:83:LYS:HE3	2:B:84:HIS:N	2.10	0.65
1:C:168:LEU:CG	1:C:172:LEU:HD11	2.20	0.65
1:C:178:THR:O	1:C:181:ARG:HB2	1.96	0.65
1:A:141:GLN:NE2	1:A:144[B]:ARG:NH1	2.45	0.65
1:C:133:TRP:CD1	4:C:283:HOH:O	2.50	0.64
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.13	0.64
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.33	0.64
1:C:14:ARG:HB2	1:C:17:LEU:HB2	1.79	0.64
1:A:138:MET:HB2	2:D:85:ASP:O	1.97	0.64
1:C:147:TRP:CB	4:C:283:HOH:O	2.46	0.63
1:A:107[B]:TRP:O	4:A:281:HOH:O	2.16	0.63
2:B:27:VAL:HG21	2:B:37:ILE:HD13	1.80	0.62
1:C:201:LEU:HD23	1:C:249:VAL:HG11	1.72	0.62
2:D:16:GLU:HG3	4:D:106:HOH:O	1.98	0.62
1:A:41:GLU:N	1:A:41:GLU:CD	2.51	0.62
2:B:1:ILE:N	2:B:1:ILE:HD13	2.12	0.62
1:A:212[B]:ASP:OD1	1:A:212[B]:ASP:C	2.37	0.62
2:D:39:MET:HE1	2:D:68:THR:HB	1.79	0.62
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.30	0.62
1:A:41:GLU:CD	1:A:41:GLU:H	2.03	0.61
2:B:27:VAL:HG21	2:B:37:ILE:CD1	2.29	0.61
1:A:227:ASP:N	1:A:227:ASP:OD2	2.33	0.61
1:A:82:LEU:HD12	1:A:87:GLN:HB2	1.82	0.61
2:D:24:ASN:OD1	2:D:67:HIS:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:O	1:C:220:ASN:C	2.40	0.60
1:C:250:PRO:O	1:C:251:LEU:O	2.20	0.59
1:C:250:PRO:O	1:C:251:LEU:C	2.40	0.59
1:C:159:TYR:HD2	1:C:160:LEU:CD1	2.15	0.59
1:A:215:LEU:HD23	1:A:261:VAL:HG22	1.84	0.59
1:C:263:HIS:CD2	1:C:265:GLY:H	2.20	0.59
1:A:218:GLN:HG2	1:A:222:GLU:HG3	1.85	0.59
1:C:99:SER:HB3	1:C:114:LEU:HD12	1.85	0.58
1:C:121:ARG:CB	1:C:121:ARG:CZ	2.81	0.58
1:A:112:GLY:HA3	1:A:160:LEU:HD23	1.86	0.58
1:A:219:LEU:CD2	1:A:220:ASN:H	2.17	0.58
1:A:48:ARG:NH2	2:B:53:ASP:OD2	2.33	0.58
1:A:138:MET:O	1:A:141:GLN:HB2	2.04	0.57
1:A:223:GLU:O	1:A:224:LEU:C	2.42	0.57
1:C:218:GLN:OE1	1:C:260:ARG:HD2	2.04	0.57
1:C:275:GLU:OE1	1:C:275:GLU:HA	2.04	0.57
1:C:14:ARG:HG3	1:C:20:PRO:HA	1.86	0.57
1:C:185:PRO:HD2	1:C:266:LEU:HD21	1.86	0.57
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.36	0.57
1:A:201:LEU:CD2	1:A:249:VAL:HG11	2.35	0.56
2:B:1:ILE:H1	2:B:1:ILE:HD13	1.69	0.56
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.40	0.56
1:A:32:GLU:CD	1:A:35:ARG:HH21	2.09	0.56
1:A:36:PHE:C	1:A:36:PHE:CD1	2.78	0.56
1:A:75:ARG:NH2	1:A:79:ARG:NH2	2.54	0.56
1:C:121:ARG:HB2	1:C:121:ARG:NH1	2.21	0.56
2:B:39:MET:CE	2:B:49:VAL:HG13	2.36	0.56
1:A:212[B]:ASP:OD1	1:A:213:ILE:N	2.38	0.55
1:A:141:GLN:NE2	1:A:144[A]:ARG:NE	2.52	0.55
1:C:130:LEU:HD22	1:C:160:LEU:HD23	1.88	0.55
1:C:41:GLU:CD	1:C:41:GLU:N	2.57	0.55
1:A:169:HIS:CE1	4:A:281:HOH:O	2.49	0.55
1:A:78:LEU:CD1	1:A:95:LEU:HB2	2.37	0.55
1:C:181:ARG:HG2	4:C:282:HOH:O	2.06	0.55
2:B:38:GLN:OE1	2:B:81:ARG:NH2	2.40	0.55
1:A:167:TRP:CZ3	1:A:170:ARG:NH1	2.74	0.55
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.37	0.55
1:C:85:TYR:O	1:C:86:ASN:HB2	2.05	0.55
1:A:141:GLN:NE2	1:A:144[B]:ARG:HH11	2.05	0.55
1:A:78:LEU:HD13	1:A:95:LEU:HB2	1.89	0.54
2:D:17:ASN:N	4:D:106:HOH:O	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:HIS:HD2	1:C:265:GLY:H	1.53	0.54
2:D:21:ASN:O	2:D:22:ILE:HD12	2.08	0.54
1:A:244:TRP:CZ2	2:B:99:MET:HG2	2.43	0.54
1:C:273:ARG:HD2	1:C:273:ARG:N	2.23	0.54
1:A:135:ALA:HB2	1:A:144[B]:ARG:HD3	1.90	0.54
1:C:185:PRO:HD2	1:C:266:LEU:HD22	1.88	0.53
1:A:206:LEU:HD23	1:A:242:GLN:HG2	1.90	0.53
2:D:38:GLN:OE1	2:D:45:LYS:HE3	2.08	0.53
1:C:274:TRP:O	1:C:275:GLU:HB2	2.08	0.53
1:A:187:ALA:HA	1:A:204:TRP:O	2.09	0.52
1:A:263:HIS:HD2	1:A:265:GLY:N	1.96	0.52
1:C:25:VAL:HG12	1:C:27:TYR:CE2	2.44	0.52
1:C:202:ARG:HD3	1:C:244:TRP:CD2	2.44	0.52
1:C:35:ARG:NH1	2:D:53:ASP:HB3	2.25	0.52
1:C:181:ARG:NH1	1:C:181:ARG:CG	2.52	0.52
1:A:41:GLU:CD	1:A:42:ASN:H	2.14	0.52
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.93	0.52
1:A:191:HIS:CD2	1:A:199:VAL:HG11	2.46	0.51
1:A:81:LEU:HD21	1:A:123:TYR:CE1	2.46	0.51
1:C:99:SER:CB	1:C:114:LEU:HD12	2.41	0.51
2:D:39:MET:CE	2:D:49:VAL:CG1	2.74	0.50
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.92	0.50
1:C:225:THR:O	1:C:227:ASP:N	2.44	0.50
1:C:255:GLN:C	1:C:257:TYR:H	2.13	0.50
1:C:121:ARG:HH22	2:D:1:ILE:N	2.10	0.50
1:A:99:SER:CB	1:A:114:LEU:HD12	2.42	0.50
1:A:106[B]:ASP:O	1:A:107[B]:TRP:CD1	2.64	0.50
1:A:106[B]:ASP:O	1:A:107[B]:TRP:CG	2.64	0.49
1:A:72:GLN:OE1	1:A:75:ARG:NH1	2.45	0.49
1:C:62:ARG:CA	1:C:65:GLN:HG2	2.41	0.49
2:B:29:GLN:HA	2:B:61:SER:OG	2.12	0.49
1:C:121:ARG:HH22	2:D:1:ILE:H1	1.61	0.49
2:D:81:ARG:HG2	2:D:81:ARG:HH11	1.78	0.49
1:A:74:PHE:HZ	1:A:97:GLN:HE21	1.62	0.48
1:C:41:GLU:OE1	1:C:41:GLU:N	2.46	0.48
1:A:274:TRP:O	1:A:275:GLU:CB	2.61	0.48
1:A:54:GLN:O	1:A:55:GLU:C	2.51	0.48
1:A:73:TRP:HE3	1:A:74:PHE:CD1	2.31	0.48
1:C:182:THR:N	4:C:282:HOH:O	2.39	0.48
1:A:81:LEU:HD21	1:A:123:TYR:CZ	2.49	0.48
1:A:92:SER:OG	2:B:34[B]:HIS:CE1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ARG:CB	1:C:17:LEU:HD23	2.41	0.48
1:C:44:ARG:NE	1:C:46:GLU:OE1	2.43	0.48
1:C:47:PRO:C	1:C:48:ARG:HG2	2.34	0.47
1:C:62:ARG:HA	1:C:65:GLN:NE2	2.27	0.47
1:A:109:LEU:CD2	1:A:161:GLU:HG2	2.43	0.47
2:B:40:LEU:CD2	2:B:45:LYS:HA	2.45	0.47
1:C:179:LEU:C	1:C:181:ARG:N	2.64	0.47
1:A:191:HIS:HB2	1:A:274:TRP:NE1	2.29	0.47
1:A:121:ARG:NH1	1:A:121:ARG:CG	2.68	0.47
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.49	0.47
2:B:88:ALA:HB1	1:C:141:GLN:HE21	1.79	0.47
2:B:89:GLU:CD	2:B:89:GLU:N	2.67	0.47
1:A:159:TYR:CD2	1:A:160:LEU:HD12	2.42	0.47
1:A:141:GLN:NE2	1:A:144[A]:ARG:CD	2.67	0.46
2:B:55:SER:HB2	2:B:63:TYR:CE2	2.50	0.46
2:D:9:VAL:HA	2:D:24:ASN:O	2.15	0.46
2:D:48:LYS:HB2	2:D:48:LYS:HE3	1.56	0.46
1:C:119:GLU:CB	2:D:1:ILE:HD13	2.45	0.46
1:C:36:PHE:C	1:C:36:PHE:CD1	2.89	0.46
1:A:88:SER:OG	1:C:86:ASN:O	2.30	0.46
1:C:3:HIS:HA	1:C:29:ASP:OD1	2.16	0.46
1:A:244:TRP:HZ2	2:B:99:MET:HG2	1.80	0.46
1:A:141:GLN:HE21	1:A:144[B]:ARG:NH1	2.13	0.46
2:B:9:VAL:HA	2:B:24:ASN:O	2.14	0.46
1:C:135:ALA:HB1	1:C:140:ALA:HB3	1.98	0.46
1:A:166:GLU:HG3	1:A:167:TRP:N	2.30	0.46
1:C:191:HIS:HD2	1:C:274:TRP:CD2	2.34	0.46
1:A:22:TYR:H	1:A:38:SER:HB2	1.81	0.45
1:A:41:GLU:N	1:A:41:GLU:OE2	2.42	0.45
1:C:84:TYR:OH	3:F:9:MET:OXT	2.20	0.45
1:A:82:LEU:HD13	4:A:277:HOH:O	2.16	0.45
1:A:252:GLY:O	1:A:254:GLU:N	2.49	0.45
1:A:75:ARG:HH21	1:A:79:ARG:NH2	2.13	0.45
1:C:218:GLN:OE1	1:C:260:ARG:NH1	2.49	0.45
1:A:129:ASP:O	1:A:131:LYS:HG3	2.16	0.45
1:C:159:TYR:HD2	1:C:160:LEU:HD13	1.79	0.45
1:A:217:TRP:N	1:A:228:MET:HE3	2.31	0.45
2:B:39:MET:HE3	2:B:49:VAL:HG13	1.98	0.45
1:C:119:GLU:HB2	2:D:1:ILE:HD13	1.99	0.45
1:C:251:LEU:O	1:C:254:GLU:HG2	2.17	0.45
1:A:223:GLU:C	1:A:224:LEU:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HG23	1:C:33:PHE:CE1	2.52	0.45
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.51	0.44
2:D:31:HIS:CD2	2:D:32:PRO:HA	2.52	0.44
2:D:83:LYS:HD3	2:D:90:PRO:HG3	2.00	0.44
1:A:210:PRO:O	1:A:263:HIS:HE1	2.00	0.44
1:C:109:LEU:CD2	1:C:161:GLU:HG2	2.47	0.44
1:A:135:ALA:HB1	1:A:140:ALA:HB1	1.98	0.44
1:C:72:GLN:OE1	1:C:75:ARG:NH1	2.46	0.44
1:A:99:SER:HB3	1:A:114:LEU:HD12	2.00	0.44
1:C:51:TRP:CZ3	1:C:52:MET:SD	3.10	0.44
2:B:89:GLU:OE2	2:B:89:GLU:N	2.48	0.44
1:C:198:GLU:HA	1:C:251:LEU:H	1.83	0.44
1:C:226:GLN:HE21	1:C:226:GLN:HA	1.81	0.44
1:A:9:GLU:HA	1:A:23:ILE:O	2.17	0.44
1:C:82:LEU:HD12	1:C:87:GLN:NE2	2.33	0.44
2:D:91:LYS:HG3	2:D:91:LYS:HZ3	1.75	0.44
1:C:159:TYR:CD2	1:C:160:LEU:HD12	2.53	0.44
1:C:82:LEU:HA	1:C:82:LEU:HD12	1.78	0.44
1:A:135:ALA:HB1	1:A:140:ALA:HB3	2.00	0.44
1:A:217:TRP:HD1	1:A:228:MET:HE2	1.82	0.43
1:C:6:ARG:HG2	1:C:8:PHE:HE2	1.82	0.43
2:D:24:ASN:OD1	2:D:67:HIS:CB	2.65	0.43
1:A:218:GLN:CD	1:A:222:GLU:HB2	2.38	0.43
1:A:211:ALA:HB1	1:A:233:THR:HG21	1.98	0.43
1:A:10:THR:HG22	1:A:11:ALA:N	2.34	0.43
1:A:27:TYR:HA	1:A:31:LYS:O	2.19	0.43
1:C:159:TYR:CD2	1:C:160:LEU:CD1	2.99	0.43
1:C:210:PRO:O	1:C:263:HIS:CE1	2.64	0.43
1:C:93:HIS:ND1	1:C:119:GLU:OE2	2.36	0.43
1:C:219:LEU:HD13	1:C:257:TYR:CZ	2.54	0.43
2:D:46:ILE:HG22	2:D:47:PRO:O	2.18	0.43
1:A:219:LEU:HD22	1:A:220:ASN:H	1.84	0.43
2:B:85:ASP:O	1:C:137:ASP:HB2	2.19	0.43
1:A:183:ASP:OD1	4:A:283:HOH:O	2.22	0.42
1:A:219:LEU:HA	1:A:256:ASN:O	2.18	0.42
1:C:257:TYR:O	1:C:273:ARG:CB	2.67	0.42
1:C:46:GLU:OE1	1:C:46:GLU:HA	2.18	0.42
1:C:62:ARG:HA	1:C:65:GLN:CG	2.46	0.42
1:C:121:ARG:NH2	2:D:1:ILE:HG12	2.34	0.42
1:A:107[A]:TRP:O	4:A:281:HOH:O	2.21	0.42
1:C:179:LEU:O	1:C:181:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:MET:HE1	2:D:67:HIS:C	2.40	0.42
1:A:110:LEU:O	1:A:111:ARG:HB3	2.19	0.42
1:A:207:GLY:C	1:A:240:THR:HB	2.39	0.42
1:A:251:LEU:CD2	1:A:252:GLY:H	2.26	0.42
1:C:4:SER:CB	1:C:102:ASP:OD1	2.63	0.42
2:D:28:THR:HG22	2:D:63:TYR:HB2	2.02	0.42
1:A:141:GLN:HE21	1:A:144[B]:ARG:HH11	1.67	0.42
1:C:58:GLU:HG2	1:C:58:GLU:H	1.58	0.42
1:A:99:SER:HB2	1:A:114:LEU:HD12	2.00	0.42
1:A:218:GLN:O	1:A:257:TYR:HA	2.20	0.42
1:A:72:GLN:HB3	4:A:282:HOH:O	2.19	0.42
1:C:215:LEU:HD23	1:C:261:VAL:HG22	2.02	0.42
1:C:235:PRO:O	2:D:10:TYR:OH	2.29	0.42
1:A:222:GLU:OE1	1:A:223:GLU:O	2.38	0.42
2:D:22:ILE:HD11	2:D:69:GLU:HG2	2.02	0.42
2:B:1:ILE:N	2:B:1:ILE:CD1	2.81	0.42
2:B:89:GLU:H	2:B:89:GLU:CD	2.23	0.42
1:C:145[B]:ARG:NH1	1:C:149:GLN:OE1	2.53	0.42
1:C:54:GLN:O	1:C:55:GLU:C	2.57	0.41
2:D:58:LYS:HE2	2:D:58:LYS:HB3	1.79	0.41
1:A:192:HIS:HA	1:A:193:PRO:HD3	1.80	0.41
2:D:16:GLU:CA	4:D:106:HOH:O	2.54	0.41
1:A:213:ILE:HG12	1:A:214:THR:N	2.35	0.41
1:A:231:VAL:HG23	1:A:244:TRP:H	1.86	0.41
1:A:251:LEU:O	1:A:253:LYS:N	2.53	0.41
2:B:3:LYS:NZ	2:B:61:SER:HB3	2.35	0.41
1:C:234:ARG:HH11	2:D:8:GLN:NE2	2.18	0.41
1:C:19:GLU:HA	1:C:20:PRO:HD3	1.90	0.41
1:C:223:GLU:HA	1:C:223:GLU:OE2	2.15	0.41
2:D:71:THR:HA	2:D:72:PRO:HD3	1.93	0.41
1:A:274:TRP:O	1:A:275:GLU:HB2	2.19	0.41
1:C:73:TRP:CH2	1:C:116:PHE:CE2	3.09	0.41
1:A:213:ILE:HG12	1:A:214:THR:H	1.86	0.40
1:C:129:ASP:C	1:C:129:ASP:OD2	2.60	0.40
1:C:215:LEU:HD12	1:C:243:LYS:HD3	2.04	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:D:19:LYS:NZ	4:A:283:HOH:O[1_666]	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:CE	4:A:283:HOH:O[1_666]	1.72	0.48

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	279/275 (102%)	251 (90%)	18 (6%)	10 (4%)	4	5
1	C	276/275 (100%)	246 (89%)	19 (7%)	11 (4%)	3	4
2	B	98/99 (99%)	93 (95%)	4 (4%)	1 (1%)	18	32
2	D	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
3	E	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	764/766 (100%)	692 (91%)	50 (6%)	22 (3%)	6	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	A	225	THR
1	C	220	ASN
1	C	251	LEU
1	A	17	LEU
1	A	18	GLU
1	A	196	LYS
1	A	221	GLY
2	B	85	ASP
1	C	2	PRO
1	C	17	LEU
1	C	18	GLU
1	C	227	ASP
1	C	252	GLY

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Mol	Chain	Res	Type
1	C	226	GLN
1	A	107[A]	TRP
1	A	107[B]	TRP
1	C	222	GLU
1	C	30	ASN
1	C	180	LEU
1	A	2	PRO
1	A	252	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	239/233 (103%)	213 (89%)	26 (11%)	7	14
1	C	236/233 (101%)	200 (85%)	36 (15%)	3	6
2	B	95/94 (101%)	84 (88%)	11 (12%)	6	12
2	D	94/94 (100%)	86 (92%)	8 (8%)	12	23
3	E	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	678/668 (102%)	597 (88%)	81 (12%)	6	11

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	35	ARG
1	A	38	SER
1	A	41	GLU
1	A	54	GLN
1	A	61	GLU
1	A	62	ARG
1	A	82	LEU
1	A	92	SER
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	154	GLU
1	A	166	GLU
1	A	170	ARG
1	A	181	ARG
1	A	190	THR
1	A	198	GLU
1	A	200	THR
1	A	202	ARG
1	A	219	LEU
1	A	227	ASP
1	A	231	VAL
1	A	251	LEU
1	A	253	LYS
1	A	260	ARG
1	A	266	LEU
1	A	273	ARG
2	B	16	GLU
2	B	22	ILE
2	B	38	GLN
2	B	42	ASN
2	B	48	LYS
2	B	68	THR
2	B	70	PHE
2	B	83	LYS
2	B	85	ASP
2	B	89	GLU
2	B	99	MET
1	C	17	LEU
1	C	35	ARG
1	C	38	SER
1	C	41	GLU
1	C	46	GLU
1	C	62	ARG
1	C	71	GLU
1	C	78	LEU
1	C	82	LEU
1	C	92	SER
1	C	111	ARG
1	C	138	MET
1	C	145[A]	ARG
1	C	145[B]	ARG
1	C	149	GLN

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Mol	Chain	Res	Type
1	C	160	LEU
1	C	181	ARG
1	C	196	LYS
1	C	201	LEU
1	C	212[A]	ASP
1	C	212[B]	ASP
1	C	218	GLN
1	C	223	GLU
1	C	224	LEU
1	C	225	THR
1	C	226	GLN
1	C	229	GLU
1	C	244	TRP
1	C	247	VAL
1	C	251	LEU
1	C	253	LYS
1	C	255	GLN
1	C	256	ASN
1	C	266	LEU
1	C	272	LEU
1	C	273	ARG
2	D	11	SER
2	D	38	GLN
2	D	48	LYS
2	D	50	GLU
2	D	70	PHE
2	D	85	ASP
2	D	89	GLU
2	D	91	LYS

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	141	GLN
1	A	169	HIS
1	A	174	ASN
1	A	192	HIS
1	A	218	GLN
1	A	263	HIS
2	B	17	ASN

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Mol	Chain	Res	Type
2	B	29	GLN
2	B	31	HIS
3	E	5	ASN
1	C	65	GLN
1	C	87	GLN
1	C	97	GLN
1	C	141	GLN
1	C	155	HIS
1	C	191	HIS
1	C	220	ASN
1	C	226	GLN
1	C	256	ASN
1	C	263	HIS
2	D	2	GLN
2	D	6	GLN
2	D	8	GLN
2	D	17	ASN
2	D	31	HIS
3	F	5	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, 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	275/275 (100%)	-0.26	7 (2%)	58	60	2, 15, 37, 45	15 (5%)
1	C	275/275 (100%)	-0.24	6 (2%)	62	64	2, 14, 42, 53	16 (5%)
2	B	99/99 (100%)	-0.53	0	100	100	3, 8, 19, 32	8 (8%)
2	D	99/99 (100%)	-0.45	1 (1%)	82	83	3, 8, 19, 33	9 (9%)
3	E	9/9 (100%)	-0.67	0	100	100	7, 8, 13, 14	0
3	F	9/9 (100%)	-0.39	0	100	100	9, 11, 16, 17	0
All	All	766/766 (100%)	-0.32	14 (1%)	69	70	2, 12, 36, 53	48 (6%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	THR	5.6
1	A	226	GLN	4.9
1	A	224	LEU	4.6
2	D	1	ILE	4.5
1	A	262	TYR	4.4
1	C	1	GLY	4.3
1	C	226	GLN	2.4
1	C	221	GLY	2.3
1	A	18	GLU	2.1
1	C	89	ALA	2.1
1	A	107[A]	TRP	2.1
1	C	196	LYS	2.1
1	C	225	THR	2.1
1	A	219	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.