



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:32 pm GMT

PDB ID : 3HPN
Title : Ligand recognition by A-class EPH receptors: crystal structures of the EPHA2 ligand-binding domain and the EPHA2/EPHRIN-A1 complex
Authors : Himanen, J.P.; Goldgur, Y.; Miao, H.; Myshkin, E.; Guo, H.; Buck, M.; Nguyen, M.; Rajashankar, K.R.; Wang, B.; Nikolov, D.B.
Deposited on : 2009-06-04
Resolution : 2.52 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
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

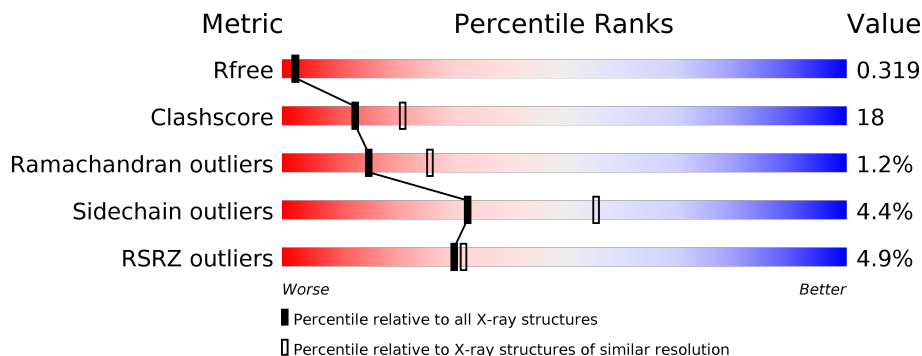
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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}	100719	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (2.54-2.50)

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 $\leq 5\%$. 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	174	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	174	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	174	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
1	D	174	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	E	174	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	F	174	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9426 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 Ephrin type-A receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	B	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	C	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	D	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	E	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	F	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			

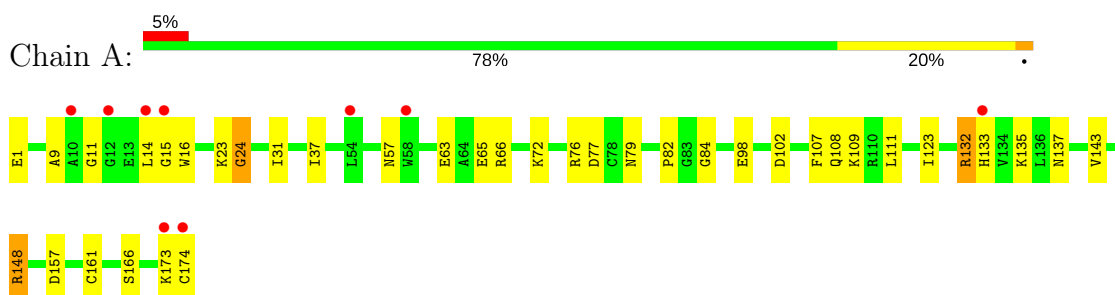
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	176	Total	O	0	0
			176	176		
2	B	190	Total	O	0	0
			190	190		
2	C	169	Total	O	0	0
			169	169		
2	D	170	Total	O	0	0
			170	170		
2	E	180	Total	O	0	0
			180	180		
2	F	147	Total	O	0	0
			147	147		

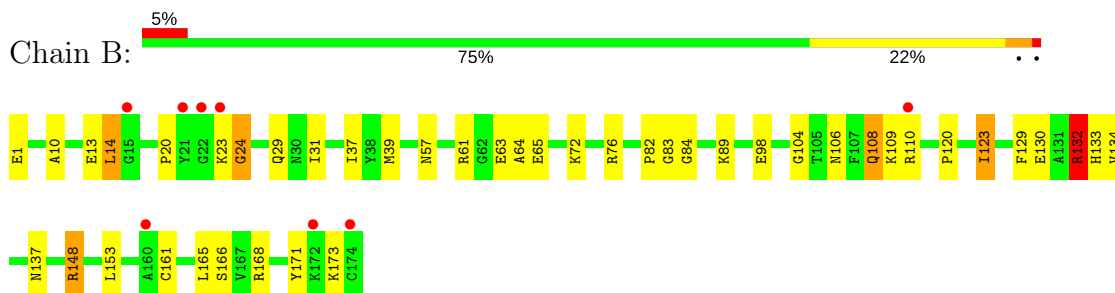
3 Residue-property plots [i](#)

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.

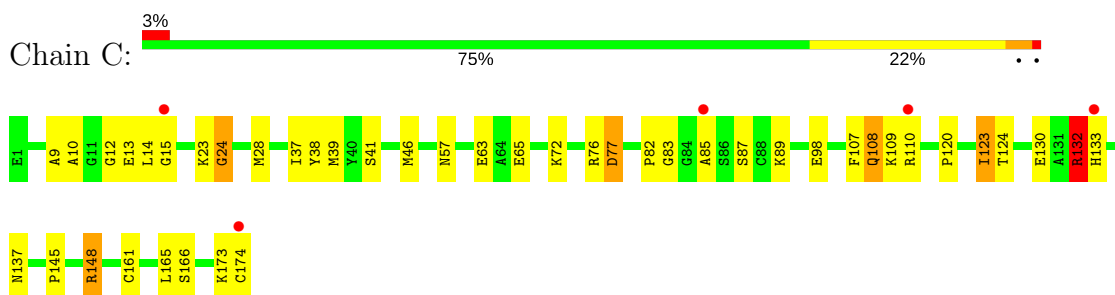
- Molecule 1: Ephrin type-A receptor 2



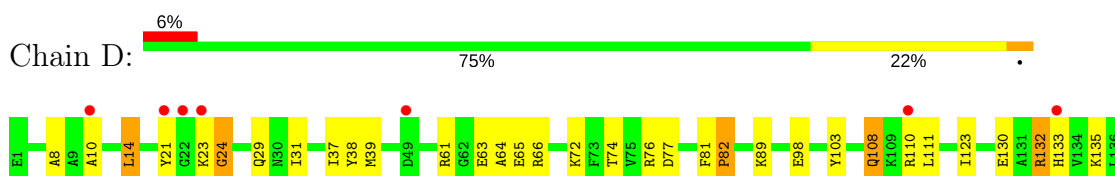
- Molecule 1: Ephrin type-A receptor 2



- Molecule 1: Ephrin type-A receptor 2

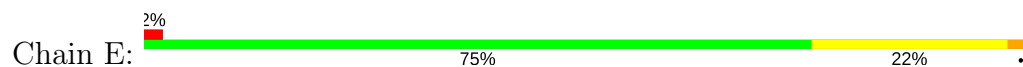


- Molecule 1: Ephrin type-A receptor 2

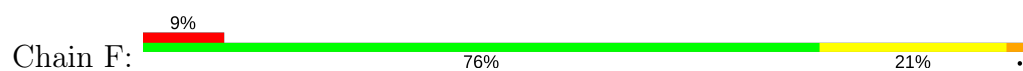




- Molecule 1: Ephrin type-A receptor 2



- Molecule 1: Ephrin type-A receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.27Å 91.19Å 91.13Å 117.14° 97.27° 100.79°	Depositor
Resolution (Å)	30.00 – 2.52 19.72 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-2.52) 80.7 (19.72-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.232 , 0.307 0.242 , 0.319	Depositor DCC
R_{free} test set	1854 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k-l,k 0.075 for h,l,-h-k-l 0.010 for -h,-l,-k 0.015 for -h,h+k+l,-l 0.014 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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	0.79	1/1433 (0.1%)	0.88	5/1940 (0.3%)
1	B	0.74	1/1433 (0.1%)	0.83	3/1940 (0.2%)
1	C	0.74	1/1433 (0.1%)	0.86	3/1940 (0.2%)
1	D	0.73	1/1433 (0.1%)	0.86	3/1940 (0.2%)
1	E	0.79	2/1433 (0.1%)	0.88	6/1940 (0.3%)
1	F	0.72	1/1433 (0.1%)	0.79	3/1940 (0.2%)
All	All	0.75	7/8598 (0.1%)	0.85	23/11640 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ARG	CZ-NH1	-9.16	1.21	1.33
1	C	132	ARG	CZ-NH1	-9.14	1.21	1.33
1	D	132	ARG	CZ-NH1	-8.69	1.21	1.33
1	E	132	ARG	CZ-NH1	-8.54	1.22	1.33
1	B	132	ARG	CZ-NH1	-8.08	1.22	1.33
1	F	132	ARG	CZ-NH1	-7.97	1.22	1.33
1	E	43	CYS	CB-SG	-5.37	1.73	1.81

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	15.71	128.15	120.30
1	E	132	ARG	NE-CZ-NH2	15.67	128.14	120.30
1	D	132	ARG	NE-CZ-NH2	15.63	128.12	120.30
1	C	132	ARG	NE-CZ-NH2	14.89	127.75	120.30
1	B	132	ARG	NE-CZ-NH2	12.39	126.50	120.30
1	F	132	ARG	NE-CZ-NH2	11.41	126.00	120.30
1	A	77	ASP	CB-CG-OD1	6.87	124.48	118.30
1	C	77	ASP	CB-CG-OD2	6.79	124.41	118.30
1	E	77	ASP	CB-CG-OD2	6.78	124.41	118.30
1	B	132	ARG	NH1-CZ-NH2	-6.59	112.15	119.40
1	C	132	ARG	NH1-CZ-NH2	-6.33	112.44	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	ASP	CB-CG-OD2	6.03	123.73	118.30
1	E	77	ASP	OD1-CG-OD2	-5.94	112.01	123.30
1	E	77	ASP	CB-CG-OD1	5.87	123.58	118.30
1	F	77	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	102	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	132	ARG	CG-CD-NE	5.47	123.29	111.80
1	A	132	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
1	E	83	GLY	N-CA-C	5.46	126.76	113.10
1	E	132	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	F	132	ARG	NH1-CZ-NH2	-5.30	113.56	119.40
1	A	77	ASP	OD1-CG-OD2	-5.28	113.27	123.30
1	D	132	ARG	NH1-CZ-NH2	-5.09	113.80	119.40

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	1399	0	1348	44	1
1	B	1399	0	1348	64	0
1	C	1399	0	1348	47	0
1	D	1399	0	1348	75	0
1	E	1399	0	1348	51	0
1	F	1399	0	1348	68	1
2	A	176	0	0	26	0
2	B	190	0	0	37	1
2	C	169	0	0	30	0
2	D	170	0	0	26	0
2	E	180	0	0	26	0
2	F	147	0	0	27	0
All	All	9426	0	8088	303	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 18.

All (303) 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:D:29:GLN:O	1:F:110:ARG:CZ	1.64	1.46
1:B:23:LYS:HE2	2:B:377:HOH:O	1.19	1.35
1:D:14:LEU:CD1	1:F:106:ASN:OD1	1.74	1.33
1:C:133:HIS:HD2	2:C:182:HOH:O	1.04	1.28
1:B:61:ARG:HG3	2:B:801:HOH:O	1.32	1.28
1:C:9:ALA:O	2:C:702:HOH:O	1.54	1.25
1:F:28:MET:HG3	2:F:674:HOH:O	1.29	1.24
1:D:38:TYR:HE2	1:F:108:GLN:NE2	1.36	1.20
1:D:14:LEU:HD11	1:F:106:ASN:OD1	1.05	1.20
1:D:29:GLN:O	1:F:110:ARG:NE	1.77	1.18
1:D:29:GLN:O	1:F:110:ARG:NH2	1.79	1.15
1:D:14:LEU:CD1	1:F:106:ASN:CG	2.15	1.14
1:D:89:LYS:HE2	2:D:767:HOH:O	1.46	1.13
1:D:23:LYS:HD3	2:D:625:HOH:O	1.51	1.08
1:B:57:ASN:HB3	2:B:194:HOH:O	1.53	1.06
1:F:106:ASN:HB2	2:F:347:HOH:O	1.54	1.06
1:A:57:ASN:HB3	2:A:833:HOH:O	1.58	1.03
1:D:14:LEU:HD12	1:F:106:ASN:CG	1.79	1.02
1:B:110:ARG:HH22	1:E:31:ILE:CD1	1.70	1.02
1:D:38:TYR:CE2	1:F:108:GLN:NE2	2.28	1.01
1:F:5:LEU:HG	2:F:261:HOH:O	1.60	1.00
1:A:31:ILE:CD1	1:D:110:ARG:HH22	1.73	1.00
1:D:21:TYR:HA	2:D:1037:HOH:O	1.60	1.00
1:E:82:PRO:O	2:E:984:HOH:O	1.80	0.99
1:D:14:LEU:HD11	1:F:106:ASN:CG	1.81	0.98
1:C:89:LYS:HG2	2:C:985:HOH:O	1.64	0.98
1:B:173:LYS:HD3	2:B:641:HOH:O	1.63	0.97
1:A:57:ASN:HB3	2:A:760:HOH:O	1.63	0.96
1:F:55:ARG:NH1	2:F:678:HOH:O	2.03	0.91
1:D:135:LYS:O	2:D:854:HOH:O	1.88	0.90
1:A:31:ILE:CG1	1:D:110:ARG:HH22	1.86	0.89
1:D:38:TYR:HE2	1:F:108:GLN:HE22	1.16	0.89
1:E:135:LYS:HE2	2:E:224:HOH:O	1.73	0.89
1:A:109:LYS:CE	2:A:389:HOH:O	2.23	0.87
1:C:15:GLY:HA2	2:C:1009:HOH:O	1.75	0.86
1:B:132:ARG:NH2	2:B:187:HOH:O	2.01	0.86
1:C:87:SER:O	2:C:985:HOH:O	1.93	0.85
2:A:728:HOH:O	1:B:133:HIS:HD2	1.60	0.85
1:A:109:LYS:HE3	2:A:389:HOH:O	1.77	0.85
1:D:38:TYR:HE2	1:F:108:GLN:CD	1.79	0.84
1:D:14:LEU:HD12	1:F:106:ASN:CB	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:HA	2:C:891:HOH:O	1.78	0.84
2:B:233:HOH:O	1:D:21:TYR:HB2	1.79	0.83
1:E:109:LYS:HD3	2:E:192:HOH:O	1.79	0.83
1:C:133:HIS:CD2	2:C:182:HOH:O	1.93	0.82
1:B:110:ARG:HH22	1:E:31:ILE:HD12	1.43	0.82
1:A:31:ILE:HG13	1:D:110:ARG:HH22	1.42	0.82
1:E:135:LYS:CE	2:E:224:HOH:O	2.27	0.82
1:A:15:GLY:O	2:A:760:HOH:O	1.99	0.81
1:C:133:HIS:CG	2:C:733:HOH:O	2.30	0.81
1:E:148:ARG:HE	1:E:148:ARG:HA	1.45	0.81
1:E:82:PRO:C	2:E:984:HOH:O	2.15	0.81
1:F:55:ARG:HB2	2:F:986:HOH:O	1.80	0.80
1:B:64:ALA:HB3	2:B:801:HOH:O	1.80	0.80
1:C:109:LYS:HD3	2:C:176:HOH:O	1.81	0.80
1:A:31:ILE:CD1	1:D:110:ARG:NH2	2.45	0.79
1:D:82:PRO:HD2	2:D:869:HOH:O	1.83	0.79
1:C:133:HIS:ND1	2:C:708:HOH:O	2.14	0.79
1:D:14:LEU:CD1	1:F:106:ASN:CB	2.61	0.78
1:E:63:GLU:OE2	1:E:173:LYS:HE2	1.82	0.78
1:F:133:HIS:CE1	2:F:776:HOH:O	2.35	0.78
1:D:137:ASN:ND2	2:D:854:HOH:O	2.16	0.78
1:D:130:GLU:CD	2:D:337:HOH:O	2.21	0.78
1:F:122:GLU:HG3	2:F:412:HOH:O	1.82	0.77
1:A:135:LYS:HE2	2:A:723:HOH:O	1.85	0.77
1:E:172:LYS:HE2	2:E:331:HOH:O	1.84	0.76
1:D:173:LYS:HB3	2:D:384:HOH:O	1.85	0.76
1:F:63:GLU:OE2	1:F:173:LYS:HE2	1.85	0.76
1:C:148:ARG:HE	1:C:148:ARG:HA	1.50	0.76
1:E:18:THR:HG23	2:E:1039:HOH:O	1.85	0.76
1:D:103:TYR:CE2	2:D:784:HOH:O	2.39	0.76
1:D:38:TYR:CE2	1:F:108:GLN:CD	2.58	0.75
1:C:98:GLU:HB3	1:C:148:ARG:HG3	1.67	0.75
1:F:55:ARG:CB	2:F:986:HOH:O	2.32	0.74
1:A:66:ARG:HD3	2:A:185:HOH:O	1.86	0.74
1:B:98:GLU:HB3	1:B:148:ARG:HG3	1.69	0.74
1:E:122:GLU:HG3	2:E:731:HOH:O	1.87	0.74
1:C:133:HIS:CD2	2:C:733:HOH:O	2.40	0.73
1:D:98:GLU:HB3	1:D:148:ARG:HG3	1.70	0.73
1:D:14:LEU:HD12	1:F:106:ASN:HB2	1.69	0.72
1:D:146:LEU:HG	2:D:990:HOH:O	1.88	0.72
1:D:63:GLU:OE2	1:D:173:LYS:HE2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:ARG:HE	1:F:148:ARG:HA	1.54	0.72
1:F:17:LEU:HD22	2:F:986:HOH:O	1.89	0.72
1:C:174:CYS:O	2:C:973:HOH:O	2.07	0.71
1:E:98:GLU:HB3	1:E:148:ARG:HG3	1.71	0.71
1:A:148:ARG:HA	1:A:148:ARG:HE	1.53	0.71
1:A:63:GLU:OE2	1:A:173:LYS:HE2	1.91	0.71
1:A:84:GLY:N	2:A:1016:HOH:O	2.22	0.70
1:C:89:LYS:HE3	2:C:185:HOH:O	1.90	0.70
1:B:110:ARG:CZ	2:B:734:HOH:O	2.38	0.70
1:B:63:GLU:OE2	1:B:173:LYS:HE2	1.91	0.70
1:B:82:PRO:HG3	2:B:305:HOH:O	1.90	0.70
1:B:20:PRO:HG3	2:B:837:HOH:O	1.90	0.70
1:F:98:GLU:HB3	1:F:148:ARG:HG3	1.75	0.69
1:E:16:TRP:N	2:E:726:HOH:O	2.24	0.69
1:C:12:GLY:N	2:C:702:HOH:O	1.67	0.69
1:B:110:ARG:NH2	1:E:31:ILE:CD1	2.52	0.69
1:D:148:ARG:HA	1:D:148:ARG:HE	1.58	0.68
1:E:108:GLN:HG3	2:E:991:HOH:O	1.92	0.68
1:B:29:GLN:H	1:D:108:GLN:HE22	1.42	0.68
1:D:29:GLN:C	1:F:110:ARG:NH2	2.46	0.67
1:B:148:ARG:HA	1:B:148:ARG:HE	1.58	0.67
1:B:110:ARG:NH2	1:E:31:ILE:HD12	2.07	0.67
1:E:174:CYS:HB2	2:E:177:HOH:O	1.94	0.67
1:A:98:GLU:HB3	1:A:148:ARG:HG3	1.77	0.67
1:C:173:LYS:O	2:C:774:HOH:O	2.13	0.67
2:A:728:HOH:O	1:B:133:HIS:CD2	2.40	0.66
1:D:89:LYS:HE3	2:D:176:HOH:O	1.95	0.65
1:A:31:ILE:HG13	1:D:110:ARG:NH2	2.11	0.65
1:C:72:LYS:HB2	1:C:166:SER:HB3	1.79	0.65
1:D:133:HIS:CE1	2:D:736:HOH:O	2.50	0.65
1:B:104:GLY:HA3	2:B:753:HOH:O	1.96	0.64
1:D:72:LYS:HB2	1:D:166:SER:HB3	1.79	0.64
1:B:57:ASN:CB	2:B:194:HOH:O	2.25	0.63
1:B:132:ARG:CZ	2:B:187:HOH:O	2.43	0.63
1:B:108:GLN:HB3	2:B:819:HOH:O	1.99	0.63
1:A:66:ARG:CD	2:A:185:HOH:O	2.44	0.62
1:A:23:LYS:O	1:A:24:GLY:O	2.17	0.62
1:A:72:LYS:HB2	1:A:166:SER:HB3	1.82	0.62
1:C:77:ASP:N	2:C:996:HOH:O	2.31	0.62
1:A:57:ASN:CB	2:A:760:HOH:O	2.31	0.62
1:F:23:LYS:HB3	2:F:190:HOH:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:HH22	1:E:31:ILE:CG1	2.12	0.61
1:D:148:ARG:HD2	2:D:989:HOH:O	1.99	0.61
1:A:107:PHE:O	2:A:607:HOH:O	2.16	0.61
1:C:57:ASN:HB3	2:C:709:HOH:O	2.00	0.61
1:E:16:TRP:O	2:E:726:HOH:O	2.16	0.61
1:B:72:LYS:HB2	1:B:166:SER:HB3	1.83	0.61
1:B:1:GLU:HG3	2:B:565:HOH:O	2.00	0.60
1:E:102:ASP:CG	2:E:255:HOH:O	2.38	0.60
1:F:57:ASN:HB3	2:F:987:HOH:O	2.03	0.59
1:E:148:ARG:CA	1:E:148:ARG:HE	2.14	0.59
1:E:81:PHE:O	1:E:82:PRO:O	2.20	0.59
1:D:29:GLN:HB3	1:F:110:ARG:HE	1.68	0.58
1:D:74:THR:HA	2:D:854:HOH:O	2.03	0.58
1:E:23:LYS:O	1:E:24:GLY:O	2.20	0.58
1:B:61:ARG:CG	2:B:801:HOH:O	2.13	0.58
1:A:157:ASP:HA	2:A:179:HOH:O	2.03	0.58
1:A:31:ILE:HD12	1:D:110:ARG:NH2	2.18	0.57
1:C:110:ARG:HB2	2:C:346:HOH:O	2.03	0.57
1:C:63:GLU:OE2	1:C:173:LYS:HE2	2.05	0.57
1:B:63:GLU:HG3	2:B:858:HOH:O	2.04	0.57
2:B:689:HOH:O	1:F:22:GLY:HA3	2.04	0.57
1:C:130:GLU:HG2	1:D:8:ALA:O	2.05	0.57
1:A:16:TRP:N	2:A:805:HOH:O	2.37	0.57
1:B:129:PHE:O	2:B:187:HOH:O	2.17	0.56
1:C:173:LYS:HB3	2:C:774:HOH:O	2.04	0.56
1:F:28:MET:CG	2:F:674:HOH:O	2.12	0.56
1:D:38:TYR:CE2	1:F:108:GLN:OE1	2.60	0.55
1:F:72:LYS:HB2	1:F:166:SER:HB3	1.88	0.55
1:F:20:PRO:HB2	2:F:232:HOH:O	2.06	0.55
1:D:29:GLN:N	1:F:110:ARG:HH21	2.05	0.55
1:F:23:LYS:HE3	2:F:449:HOH:O	2.07	0.54
1:F:15:GLY:HA3	2:F:987:HOH:O	2.06	0.54
1:C:28:MET:HE3	1:C:41:SER:HB3	1.90	0.54
1:F:55:ARG:HB3	2:F:986:HOH:O	2.04	0.54
1:B:168:ARG:NH2	2:B:446:HOH:O	2.40	0.53
1:B:84:GLY:N	2:B:332:HOH:O	2.41	0.53
1:E:133:HIS:HD2	2:E:181:HOH:O	1.91	0.53
1:B:89:LYS:HE3	2:B:228:HOH:O	2.07	0.53
1:F:76:ARG:HB3	1:F:161:CYS:HB3	1.89	0.53
1:B:173:LYS:CD	2:B:641:HOH:O	2.36	0.53
1:E:76:ARG:HB2	1:F:33:ASN:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:CYS:SG	2:E:578:HOH:O	2.52	0.53
1:D:172:LYS:HE2	2:D:260:HOH:O	2.09	0.52
1:C:107:PHE:HD2	2:C:803:HOH:O	1.92	0.52
1:E:72:LYS:HB2	1:E:166:SER:HB3	1.90	0.52
1:B:110:ARG:HH22	1:E:31:ILE:HD11	1.69	0.52
1:E:172:LYS:CE	2:E:331:HOH:O	2.52	0.52
1:B:148:ARG:CA	1:B:148:ARG:HE	2.23	0.52
1:B:76:ARG:HB3	1:B:161:CYS:HB3	1.91	0.51
1:E:102:ASP:OD2	2:E:255:HOH:O	2.19	0.51
1:F:28:MET:CB	2:F:674:HOH:O	2.54	0.51
1:D:173:LYS:O	2:D:384:HOH:O	2.19	0.51
1:C:123:ILE:HG23	2:C:996:HOH:O	2.10	0.51
1:B:20:PRO:CG	2:B:837:HOH:O	2.52	0.51
1:B:83:GLY:HA3	2:B:1019:HOH:O	2.10	0.51
1:F:133:HIS:HE1	2:F:776:HOH:O	1.83	0.51
1:A:109:LYS:NZ	2:A:389:HOH:O	2.35	0.50
1:D:133:HIS:ND1	2:D:736:HOH:O	2.35	0.50
1:A:148:ARG:CA	1:A:148:ARG:HE	2.23	0.50
1:D:21:TYR:CA	2:D:1037:HOH:O	2.33	0.50
1:B:134:VAL:HB	2:B:177:HOH:O	2.12	0.50
1:E:76:ARG:HB3	1:E:161:CYS:HB3	1.93	0.50
1:D:108:GLN:HA	2:D:186:HOH:O	2.12	0.49
1:D:76:ARG:HB3	1:D:161:CYS:HB3	1.94	0.49
1:A:76:ARG:HB3	1:A:161:CYS:HB3	1.93	0.49
1:C:124:THR:N	2:C:996:HOH:O	2.44	0.49
1:E:133:HIS:CD2	2:E:181:HOH:O	2.64	0.49
1:F:109:LYS:HD3	2:F:820:HOH:O	2.12	0.49
1:A:23:LYS:O	1:A:24:GLY:C	2.49	0.49
1:C:132:ARG:HD3	1:D:165:LEU:O	2.13	0.49
1:A:31:ILE:HD11	1:D:110:ARG:HH22	1.69	0.49
1:A:173:LYS:NZ	2:A:902:HOH:O	2.04	0.48
1:B:29:GLN:H	1:D:108:GLN:NE2	2.09	0.48
1:C:133:HIS:CE1	2:C:708:HOH:O	2.64	0.48
1:F:148:ARG:HE	1:F:148:ARG:CA	2.20	0.48
1:B:133:HIS:CE1	2:B:300:HOH:O	2.67	0.48
1:C:132:ARG:HD3	1:D:165:LEU:HB3	1.95	0.48
1:B:108:GLN:HE22	1:F:29:GLN:H	1.60	0.48
1:A:109:LYS:HE3	2:A:186:HOH:O	2.12	0.48
1:A:111:LEU:HB3	2:A:848:HOH:O	2.13	0.48
1:B:98:GLU:HB3	1:B:148:ARG:CG	2.41	0.48
1:F:65:GLU:HG2	2:F:782:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LYS:NZ	2:B:406:HOH:O	2.33	0.47
1:C:76:ARG:HB3	1:C:161:CYS:HB3	1.95	0.47
1:A:143:VAL:HG13	2:A:392:HOH:O	2.15	0.47
1:D:148:ARG:CA	1:D:148:ARG:HE	2.22	0.47
1:E:57:ASN:HB2	2:E:179:HOH:O	2.15	0.47
1:B:132:ARG:NE	2:B:187:HOH:O	2.48	0.47
1:A:98:GLU:HB3	1:A:148:ARG:CG	2.44	0.47
1:D:14:LEU:CD1	1:F:106:ASN:HB2	2.38	0.47
1:B:108:GLN:HA	2:B:270:HOH:O	2.15	0.47
1:B:29:GLN:NE2	1:D:111:LEU:HD21	2.30	0.47
1:B:110:ARG:HH22	1:E:31:ILE:HG13	1.79	0.46
1:F:39:MET:HE2	1:F:39:MET:HB3	1.79	0.46
1:D:39:MET:HE2	1:D:39:MET:HB3	1.83	0.46
1:A:174:CYS:HB2	2:A:868:HOH:O	2.15	0.46
1:B:173:LYS:HG2	2:B:193:HOH:O	2.15	0.46
1:F:107:PHE:HA	2:F:678:HOH:O	2.16	0.46
1:F:30:ASN:ND2	1:F:39:MET:HE3	2.31	0.46
1:C:82:PRO:HB3	2:C:1007:HOH:O	2.16	0.46
1:C:148:ARG:CA	1:C:148:ARG:HE	2.21	0.46
1:B:39:MET:HE2	1:B:39:MET:HB3	1.85	0.46
1:B:64:ALA:HB2	1:B:171:TYR:CD2	2.51	0.45
1:C:46:MET:SD	2:C:1006:HOH:O	2.61	0.45
1:F:39:MET:HG3	2:F:674:HOH:O	2.14	0.45
1:A:72:LYS:HA	1:A:137:ASN:O	2.16	0.45
1:E:98:GLU:HB3	1:E:148:ARG:CG	2.43	0.45
1:A:65:GLU:OE1	2:A:977:HOH:O	2.21	0.45
1:B:23:LYS:O	1:B:24:GLY:C	2.54	0.45
1:C:12:GLY:CA	2:C:702:HOH:O	2.45	0.45
1:E:72:LYS:HA	1:E:137:ASN:O	2.17	0.45
1:E:23:LYS:O	1:E:24:GLY:C	2.54	0.45
1:F:168:ARG:NE	2:F:550:HOH:O	2.50	0.45
1:C:108:GLN:HE21	1:C:108:GLN:HB3	1.52	0.45
1:B:13:GLU:HG2	1:B:14:LEU:HD13	1.99	0.44
1:D:23:LYS:O	1:D:24:GLY:C	2.55	0.44
1:D:66:ARG:HA	2:D:990:HOH:O	2.17	0.44
1:C:83:GLY:N	2:C:231:HOH:O	2.46	0.44
1:F:30:ASN:ND2	1:F:39:MET:CE	2.81	0.44
1:A:79:ASN:HB3	2:A:206:HOH:O	2.17	0.44
1:D:29:GLN:C	1:F:110:ARG:HH21	2.18	0.44
1:C:109:LYS:HG3	2:C:187:HOH:O	2.18	0.44
1:D:110:ARG:HG2	2:D:662:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:HA	1:B:130:GLU:HG2	2.00	0.44
1:B:173:LYS:CG	2:B:193:HOH:O	2.66	0.44
1:B:108:GLN:HB3	1:B:108:GLN:HE21	1.67	0.43
1:C:39:MET:HB3	1:C:165:LEU:HD13	2.01	0.43
1:C:72:LYS:HA	1:C:137:ASN:O	2.19	0.43
1:A:16:TRP:CD1	1:A:16:TRP:N	2.86	0.43
1:F:173:LYS:CG	2:F:192:HOH:O	2.66	0.43
1:B:137:ASN:HB3	2:B:199:HOH:O	2.18	0.43
1:B:120:PRO:HG2	1:B:123:ILE:HD12	2.01	0.43
1:C:23:LYS:O	1:C:24:GLY:C	2.55	0.43
1:D:23:LYS:HB2	2:D:1012:HOH:O	2.19	0.43
1:E:39:MET:HE2	1:E:165:LEU:CD1	2.49	0.43
1:F:122:GLU:CG	2:F:412:HOH:O	2.54	0.43
1:D:39:MET:HB3	1:D:165:LEU:HD13	2.01	0.43
1:E:27:LEU:HD13	1:E:40:TYR:CE1	2.53	0.43
1:E:65:GLU:O	1:E:145:PRO:HA	2.18	0.43
1:C:120:PRO:HG2	1:C:123:ILE:HD12	2.00	0.42
1:D:148:ARG:CZ	2:D:194:HOH:O	2.67	0.42
1:F:107:PHE:CA	2:F:678:HOH:O	2.67	0.42
1:B:23:LYS:CE	2:B:377:HOH:O	2.07	0.42
1:B:82:PRO:HD2	2:B:937:HOH:O	2.19	0.42
2:B:181:HOH:O	1:F:28:MET:HB3	2.18	0.42
1:A:133:HIS:HE1	2:A:551:HOH:O	2.02	0.42
2:B:689:HOH:O	1:F:22:GLY:CA	2.64	0.42
1:F:28:MET:HB2	2:F:674:HOH:O	2.17	0.42
1:B:29:GLN:HE21	1:B:31:ILE:HG12	1.85	0.42
1:D:81:PHE:O	1:D:82:PRO:O	2.37	0.42
1:E:110:ARG:CZ	2:E:806:HOH:O	2.68	0.42
1:B:72:LYS:HA	1:B:137:ASN:O	2.20	0.42
1:A:82:PRO:HD2	2:A:713:HOH:O	2.20	0.42
1:D:174:CYS:HB3	2:D:185:HOH:O	2.19	0.42
1:E:36:PRO:HD3	2:E:798:HOH:O	2.20	0.42
1:F:29:GLN:HE21	1:F:31:ILE:HG12	1.85	0.42
1:E:66:ARG:NH2	2:E:372:HOH:O	2.53	0.41
1:C:85:ALA:HA	2:C:804:HOH:O	2.21	0.41
1:A:9:ALA:O	1:A:11:GLY:N	2.51	0.41
1:C:98:GLU:HB3	1:C:148:ARG:CG	2.43	0.41
1:E:110:ARG:NE	2:E:806:HOH:O	2.54	0.41
1:C:38:TYR:OH	2:C:741:HOH:O	2.22	0.41
1:E:107:PHE:C	1:E:108:GLN:HG2	2.40	0.41
1:C:65:GLU:O	1:C:145:PRO:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:GLU:HB3	1:F:148:ARG:CG	2.49	0.41
1:D:108:GLN:HB3	2:D:596:HOH:O	2.20	0.41
1:A:1:GLU:HB2	2:A:788:HOH:O	2.20	0.41
1:D:64:ALA:HB2	1:D:171:TYR:CD2	2.56	0.41
1:E:108:GLN:N	2:E:793:HOH:O	2.49	0.41
1:F:120:PRO:HG2	1:F:123:ILE:HD12	2.02	0.41
1:B:39:MET:HB3	1:B:165:LEU:HD13	2.03	0.40
1:B:106:ASN:ND2	1:F:27:LEU:HD23	2.36	0.40
1:F:72:LYS:HA	1:F:137:ASN:O	2.21	0.40
1:D:29:GLN:HE21	1:D:31:ILE:HG12	1.87	0.40
1:E:39:MET:HB3	1:E:165:LEU:HD13	2.02	0.40
1:E:39:MET:HE2	1:E:39:MET:HB3	1.90	0.40
1:E:63:GLU:N	2:E:496:HOH:O	2.52	0.40
1:D:65:GLU:O	1:D:145:PRO:HA	2.21	0.40
1:D:61:ARG:NH2	2:D:202:HOH:O	2.54	0.40
1:E:58:TRP:HE3	2:E:255:HOH:O	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:B:440:HOH:O	2:B:954:HOH:O[1_455]	1.95	0.25
1:A:174:CYS:CA	1:F:174:CYS:O[1_456]	2.01	0.19

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	172/174 (99%)	158 (92%)	13 (8%)	1 (1%)	28	47
1	B	172/174 (99%)	161 (94%)	9 (5%)	2 (1%)	15	26
1	C	172/174 (99%)	159 (92%)	11 (6%)	2 (1%)	15	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	172/174 (99%)	157 (91%)	12 (7%)	3 (2%)	11	17
1	E	172/174 (99%)	158 (92%)	11 (6%)	3 (2%)	11	17
1	F	172/174 (99%)	159 (92%)	12 (7%)	1 (1%)	28	47
All	All	1032/1044 (99%)	952 (92%)	68 (7%)	12 (1%)	15	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	E	24	GLY
1	E	82	PRO
1	B	24	GLY
1	C	24	GLY
1	D	24	GLY
1	E	83	GLY
1	F	24	GLY
1	C	10	ALA
1	D	10	ALA
1	B	10	ALA
1	D	82	PRO

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	150/150 (100%)	144 (96%)	6 (4%)	36	60
1	B	150/150 (100%)	142 (95%)	8 (5%)	26	46
1	C	150/150 (100%)	144 (96%)	6 (4%)	36	60
1	D	150/150 (100%)	144 (96%)	6 (4%)	36	60
1	E	150/150 (100%)	143 (95%)	7 (5%)	30	52
1	F	150/150 (100%)	143 (95%)	7 (5%)	30	52
All	All	900/900 (100%)	860 (96%)	40 (4%)	33	55

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	37	ILE
1	A	108	GLN
1	A	123	ILE
1	A	132	ARG
1	A	148	ARG
1	B	14	LEU
1	B	37	ILE
1	B	65	GLU
1	B	108	GLN
1	B	123	ILE
1	B	132	ARG
1	B	148	ARG
1	B	153	LEU
1	C	14	LEU
1	C	37	ILE
1	C	108	GLN
1	C	123	ILE
1	C	132	ARG
1	C	148	ARG
1	D	14	LEU
1	D	37	ILE
1	D	108	GLN
1	D	123	ILE
1	D	132	ARG
1	D	148	ARG
1	E	14	LEU
1	E	37	ILE
1	E	108	GLN
1	E	123	ILE
1	E	132	ARG
1	E	148	ARG
1	E	153	LEU
1	F	14	LEU
1	F	37	ILE
1	F	65	GLU
1	F	108	GLN
1	F	123	ILE
1	F	132	ARG
1	F	148	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	ASN
1	A	44	ASN
1	A	79	ASN
1	A	106	ASN
1	A	108	GLN
1	A	133	HIS
1	B	19	HIS
1	B	29	GLN
1	B	44	ASN
1	B	79	ASN
1	B	106	ASN
1	B	108	GLN
1	B	133	HIS
1	C	29	GLN
1	C	30	ASN
1	C	33	ASN
1	C	44	ASN
1	C	79	ASN
1	C	106	ASN
1	C	108	GLN
1	C	133	HIS
1	D	44	ASN
1	D	79	ASN
1	D	106	ASN
1	D	108	GLN
1	E	29	GLN
1	E	33	ASN
1	E	44	ASN
1	E	79	ASN
1	E	106	ASN
1	E	108	GLN
1	E	133	HIS
1	F	30	ASN
1	F	33	ASN
1	F	44	ASN
1	F	79	ASN
1	F	106	ASN
1	F	108	GLN
1	F	133	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	174/174 (100%)	0.34	9 (5%) 28 29	2, 2, 3, 4	0
1	B	174/174 (100%)	0.43	8 (4%) 33 35	2, 2, 3, 4	0
1	C	174/174 (100%)	0.29	5 (2%) 52 55	2, 2, 2, 4	0
1	D	174/174 (100%)	0.45	10 (5%) 24 26	2, 2, 3, 4	0
1	E	174/174 (100%)	0.32	4 (2%) 61 63	2, 2, 2, 4	0
1	F	174/174 (100%)	0.64	15 (8%) 11 11	2, 2, 2, 3	0
All	All	1044/1044 (100%)	0.41	51 (4%) 30 32	2, 2, 3, 4	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	CYS	8.5
1	D	174	CYS	8.4
1	B	174	CYS	8.4
1	A	174	CYS	8.1
1	F	174	CYS	7.9
1	E	174	CYS	6.9
1	F	21	TYR	5.9
1	E	10	ALA	5.5
1	D	10	ALA	5.3
1	F	22	GLY	4.8
1	A	15	GLY	4.5
1	D	22	GLY	4.3
1	D	21	TYR	4.2
1	D	23	LYS	4.1
1	F	108	GLN	4.1
1	F	101	LEU	4.0
1	B	21	TYR	3.9
1	F	106	ASN	3.5
1	D	110	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	22	GLY	3.4
1	B	110	ARG	3.3
1	F	173	LYS	3.3
1	A	14	LEU	3.2
1	B	15	GLY	3.2
1	E	110	ARG	3.1
1	F	102	ASP	3.1
1	A	12	GLY	3.1
1	A	173	LYS	3.1
1	F	103	TYR	2.9
1	A	10	ALA	2.8
1	E	11	GLY	2.7
1	F	15	GLY	2.7
1	F	110	ARG	2.7
1	D	133	HIS	2.7
1	C	15	GLY	2.6
1	C	85	ALA	2.6
1	B	23	LYS	2.6
1	B	172	LYS	2.6
1	F	63	GLU	2.4
1	C	133	HIS	2.4
1	A	58	TRP	2.3
1	A	54	LEU	2.2
1	F	46	MET	2.2
1	A	133	HIS	2.2
1	F	133	HIS	2.1
1	D	49	ASP	2.1
1	B	160	ALA	2.1
1	D	151	PHE	2.1
1	F	131	ALA	2.0
1	D	162	VAL	2.0
1	C	110	ARG	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.