Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:58 am BST

PDB ID	:	2V7N
Title	:	Unusual twinning in crystals of the CitS binding antibody Fab fragment f3p4
Authors	:	Frey, D.; Huber, T.; Plueckthun, A.; Gruetter, M.G.
Deposited on	:	2007-07-31
Resolution	:	1.92 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 ①) were used in the production of this report:

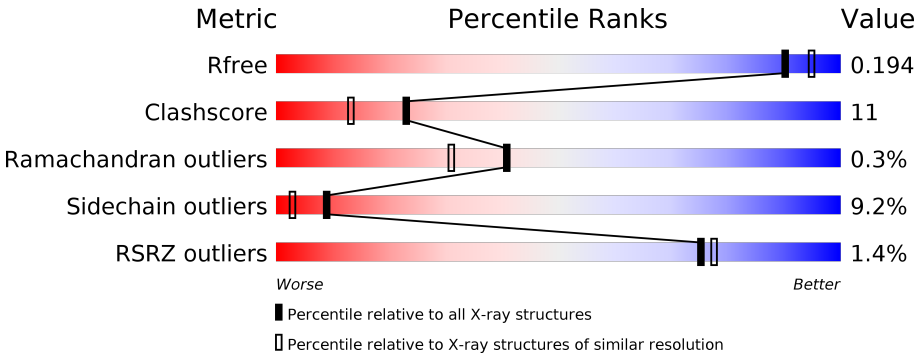
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	215	71% 23%
1	C	215	71% 24%
1	E	215	69% 25% 5%
1	G	215	% 74% 23%
2	B	229	70% 21% 7%
2	D	229	4% 68% 21% 7%

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Mol	Chain	Length	Quality of chain
2	F	229	2% 63% 25% 7%
2	H	229	2% 66% 22% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13417 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 IMMUNOGLOBULIN LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1631	1019	275	333	4			
1	C	212	Total	C	N	O	S	0	0	0
			1627	1017	274	332	4			
1	E	213	Total	C	N	O	S	0	0	0
			1631	1019	275	333	4			
1	G	212	Total	C	N	O	S	0	0	0
			1627	1017	274	332	4			

- Molecule 2 is a protein called IMMUNOGLOBULIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1598	1011	272	309	6			
2	D	213	Total	C	N	O	S	0	0	0
			1595	1010	272	307	6			
2	F	212	Total	C	N	O	S	0	0	0
			1586	1005	270	305	6			
2	H	211	Total	C	N	O	S	0	0	0
			1582	1003	269	304	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		
3	B	58	Total	O	0	0
			58	58		
3	C	80	Total	O	0	0
			80	80		
3	D	61	Total	O	0	0
			61	61		

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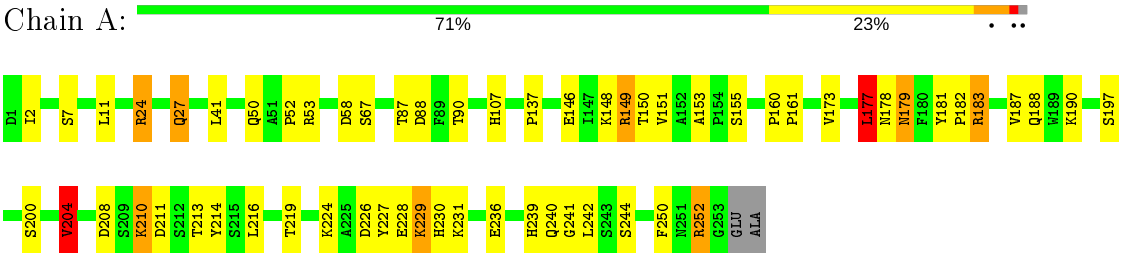
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	64	Total O 64 64	0	0
3	F	51	Total O 51 51	0	0
3	G	80	Total O 80 80	0	0
3	H	61	Total O 61 61	0	0

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.

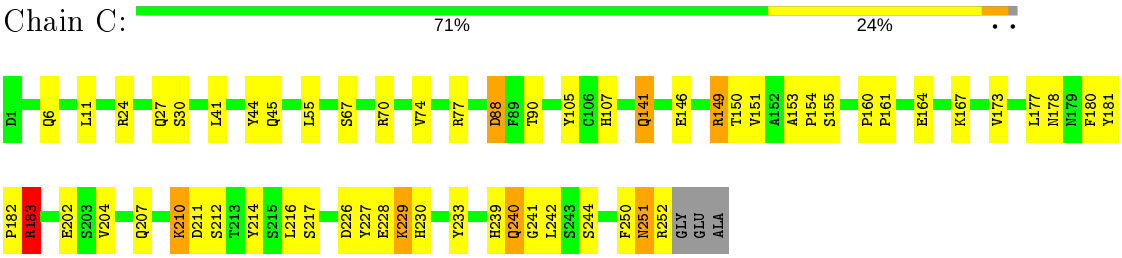
- Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

Chain A:



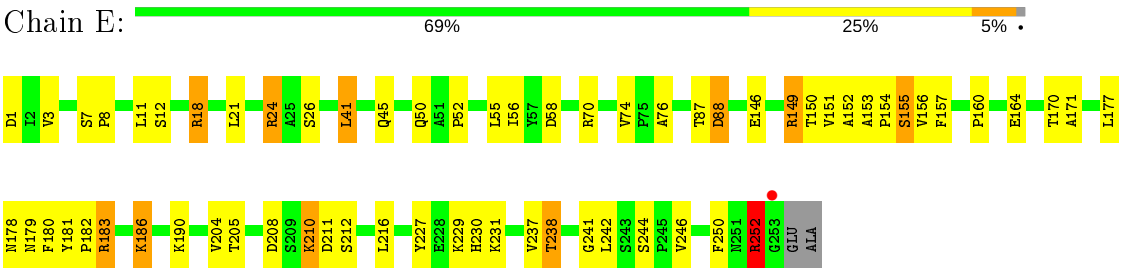
- Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

Chain C:



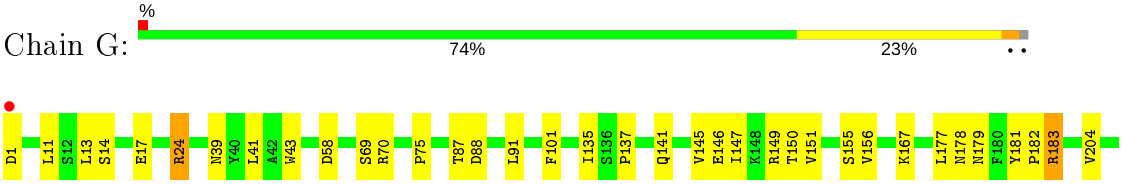
- Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

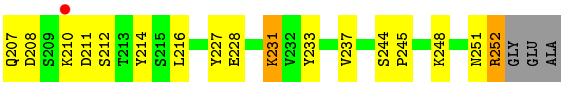
Chain E:



- Molecule 1: IMMUNOGLOBULIN LIGHT CHAIN

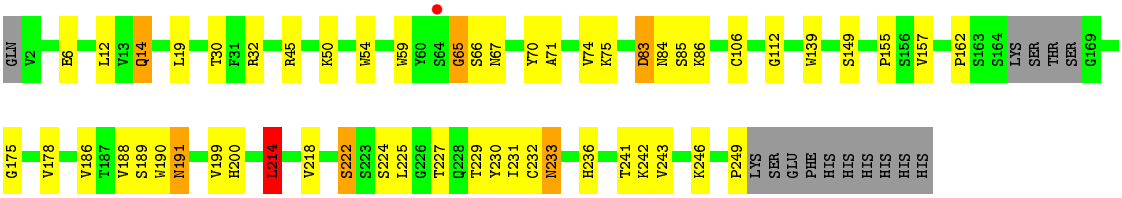
Chain G:





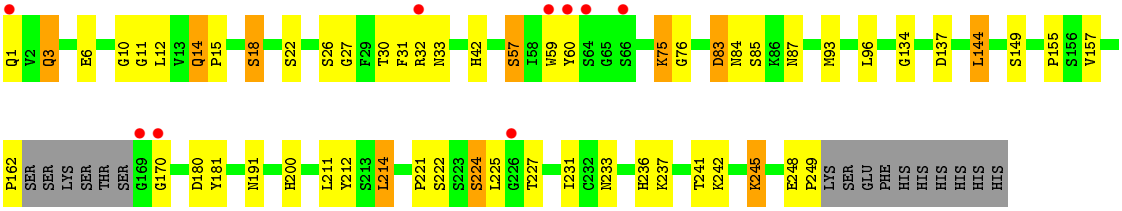
• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

Chain B:



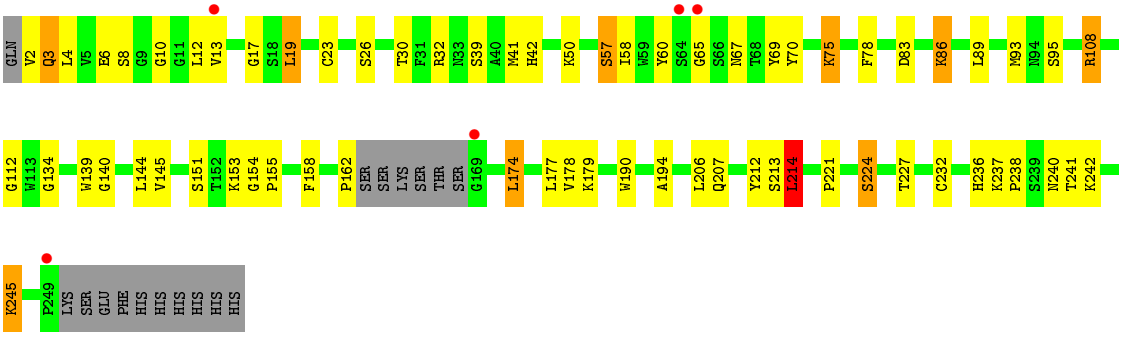
• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

Chain D:



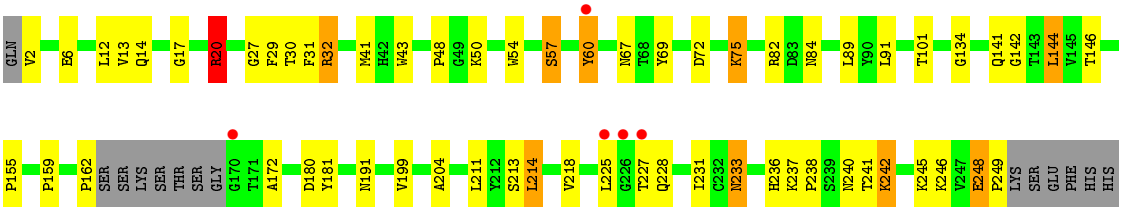
• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

Chain F:



• Molecule 2: IMMUNOGLOBULIN HEAVY CHAIN

Chain H:



HIS
HIS
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HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.79Å 185.92Å 102.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.92 29.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.1 (15.00-1.92) 96.7 (29.99-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 1.91Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.155 , 0.202 0.151 , 0.194	Depositor DCC
R_{free} test set	4240 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.389 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13417	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.24% 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	0.39	0/1667	1.00	6/2267 (0.3%)
1	C	0.38	0/1663	1.03	5/2262 (0.2%)
1	E	0.39	0/1667	1.04	5/2267 (0.2%)
1	G	0.39	0/1663	1.02	4/2262 (0.2%)
2	B	0.37	0/1639	1.02	6/2234 (0.3%)
2	D	0.37	0/1636	0.98	5/2230 (0.2%)
2	F	0.37	0/1627	1.04	6/2218 (0.3%)
2	H	0.36	0/1623	0.97	3/2213 (0.1%)
All	All	0.38	0/13185	1.01	40/17953 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	ARG	CD-NE-CZ	14.47	143.87	123.60
1	E	252	ARG	NE-CZ-NH1	-10.07	115.27	120.30
2	F	214	LEU	CA-CB-CG	9.60	137.38	115.30
1	A	252	ARG	NE-CZ-NH1	-8.86	115.87	120.30
2	B	83	ASP	CB-CG-OD2	8.74	126.17	118.30
1	E	183	ARG	CD-NE-CZ	8.48	135.47	123.60
2	B	83	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	G	183	ARG	CD-NE-CZ	8.00	134.81	123.60
2	B	45	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	H	214	LEU	CA-CB-CG	7.86	133.38	115.30
1	C	183	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	E	183	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	B	70	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	D	83	ASP	CB-CG-OD1	6.98	124.58	118.30
1	C	183	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	252	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	G	183	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	D	214	LEU	CA-CB-CG	6.55	130.37	115.30
2	H	144	LEU	CB-CG-CD2	6.54	122.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	183	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	F	60	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	204	VAL	CA-CB-CG1	5.97	119.86	110.90
2	B	214	LEU	CA-CB-CG	5.94	128.96	115.30
1	E	41	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	183	ARG	CD-NE-CZ	5.60	131.44	123.60
2	F	60	TYR	CB-CG-CD1	5.59	124.35	121.00
2	D	137	ASP	CB-CG-OD1	5.46	123.21	118.30
2	D	225	LEU	CA-C-N	5.44	127.08	116.20
2	F	86	LYS	CA-CB-CG	5.44	125.36	113.40
2	F	108	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	84	ASN	CB-CG-OD1	5.25	132.09	121.60
1	E	183	ARG	CA-CB-CG	5.23	124.90	113.40
1	C	105	TYR	CB-CG-CD2	-5.14	117.92	121.00
2	H	20	ARG	CA-CB-CG	5.14	124.71	113.40
1	A	11	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	177	LEU	CB-CG-CD2	-5.12	102.30	111.00
2	F	83	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	177	LEU	CA-CB-CG	5.09	127.00	115.30
1	G	177	LEU	CA-CB-CG	5.04	126.89	115.30
2	D	212	TYR	CB-CG-CD2	-5.02	117.99	121.00

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	1631	0	1580	35	0
1	C	1627	0	1577	39	0
1	E	1631	0	1580	51	0
1	G	1627	0	1577	27	0
2	B	1598	0	1549	38	0
2	D	1595	0	1550	28	0
2	F	1586	0	1539	40	0
2	H	1582	0	1536	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	85	0	0	1	0
3	B	58	0	0	2	0
3	C	80	0	0	1	0
3	D	61	0	0	1	0
3	E	64	0	0	3	0
3	F	51	0	0	1	0
3	G	80	0	0	0	0
3	H	61	0	0	1	0
All	All	13417	0	12488	288	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 11.

All (288) 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)
2:B:229:THR:HG23	2:B:246:LYS:HE3	1.55	0.88
1:C:6:GLN:H	1:C:141:GLN:HE22	1.20	0.87
1:G:204:VAL:HG22	1:G:216:LEU:HD12	1.59	0.84
2:F:236:HIS:HB3	2:F:241:THR:HB	1.61	0.83
1:C:164:GLU:HA	1:C:167:LYS:HD3	1.60	0.81
2:H:162:PRO:HG2	2:H:249:PRO:HA	1.63	0.80
1:A:2:ILE:HG12	1:A:27:GLN:HG3	1.63	0.80
1:E:1:ASP:HB3	3:E:2027:HOH:O	1.83	0.76
2:F:3:GLN:HG2	2:F:26:SER:OG	1.87	0.74
1:C:45:GLN:HB2	1:C:55:LEU:HD11	1.68	0.74
2:D:162:PRO:HG2	2:D:249:PRO:HG3	1.70	0.73
2:H:155:PRO:HD2	2:H:241:THR:HG21	1.71	0.73
1:E:177:LEU:HD11	1:E:237:VAL:HG21	1.68	0.73
2:B:191:ASN:ND2	2:B:231:ILE:H	1.86	0.72
1:E:186:LYS:HG2	1:E:238:THR:OG1	1.90	0.71
2:F:179:LYS:HE2	2:F:207:GLN:OE1	1.91	0.71
1:E:156:VAL:HG22	1:E:177:LEU:HD13	1.71	0.70
2:B:178:VAL:HB	2:B:214:LEU:HD23	1.74	0.70
1:C:151:VAL:HG11	1:C:240:GLN:HG2	1.74	0.69
2:B:59:TRP:HB2	2:B:66:SER:HA	1.76	0.68
2:D:1:GLN:O	2:D:27:GLY:HA3	1.92	0.68
2:B:14:GLN:NE2	2:B:149:SER:HA	2.10	0.67
2:B:199:VAL:HG22	2:B:218:VAL:HG22	1.76	0.67
2:D:170:GLY:O	2:D:221:PRO:HA	1.94	0.67
2:F:6:GLU:OE2	2:F:140:GLY:HA3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:ASP:HB3	1:G:211:ASP:OD1	1.94	0.66
2:F:155:PRO:HD2	2:F:241:THR:HG21	1.77	0.65
2:F:4:LEU:HD22	2:F:23:CYS:SG	2.36	0.65
1:A:151:VAL:HG22	1:A:240:GLN:HE21	1.62	0.65
1:C:226:ASP:HA	1:C:229:LYS:HE2	1.77	0.65
1:E:183:ARG:NH2	1:E:204:VAL:HG21	2.11	0.65
1:A:239:HIS:CD2	1:A:241:GLY:H	2.15	0.64
2:H:236:HIS:HB3	2:H:241:THR:HB	1.79	0.64
2:D:14:GLN:NE2	2:D:149:SER:HA	2.14	0.63
2:D:191:ASN:HD21	2:D:231:ILE:H	1.46	0.63
2:D:3:GLN:HG2	2:D:26:SER:OG	1.97	0.63
1:G:146:GLU:HG3	1:G:214:TYR:OH	1.98	0.63
1:C:149:ARG:HD3	1:C:150:THR:O	1.98	0.63
1:E:24:ARG:NH2	1:E:88:ASP:HB2	2.14	0.63
2:D:32:ARG:NH1	2:D:84:ASN:HB3	2.14	0.62
1:A:229:LYS:HG2	1:A:230:HIS:CE1	2.33	0.62
2:H:180:ASP:HB3	2:H:211:LEU:HD13	1.82	0.62
2:D:191:ASN:ND2	2:D:231:ILE:H	1.98	0.62
1:A:161:PRO:HD3	1:A:173:VAL:HG22	1.82	0.62
2:B:191:ASN:HD21	2:B:231:ILE:H	1.48	0.62
1:C:226:ASP:OD1	1:C:229:LYS:HE3	2.00	0.61
1:A:178:ASN:HD21	2:B:200:HIS:CD2	2.18	0.61
1:C:204:VAL:HG22	1:C:216:LEU:HD12	1.82	0.61
2:H:13:VAL:HG12	2:H:14:GLN:O	2.01	0.61
2:F:206:LEU:HD13	2:F:212:TYR:CZ	2.36	0.60
2:D:157:VAL:O	2:D:245:LYS:HE2	2.02	0.60
1:G:231:LYS:HE3	1:G:251:ASN:HB3	1.83	0.60
2:H:60:TYR:HA	2:H:82:ARG:NH1	2.17	0.60
2:H:82:ARG:HE	2:H:84:ASN:HD21	1.49	0.59
2:H:30:THR:HG22	2:H:32:ARG:HG3	1.84	0.59
2:F:42:HIS:CD2	2:F:57:SER:HB3	2.37	0.59
1:C:227:TYR:CZ	1:C:252:ARG:HG3	2.36	0.59
2:B:157:VAL:HG13	2:B:178:VAL:HG22	1.84	0.59
2:D:75:LYS:HE3	2:D:76:GLY:H	1.68	0.59
1:E:177:LEU:HD11	1:E:237:VAL:HG11	1.84	0.59
1:E:242:LEU:HD22	1:E:246:VAL:HG23	1.83	0.59
1:E:45:GLN:HB2	1:E:55:LEU:HD11	1.83	0.59
2:F:75:LYS:HE2	2:F:75:LYS:HA	1.85	0.59
1:A:208:ASP:HB3	1:A:211:ASP:OD1	2.03	0.59
2:B:191:ASN:HD21	2:B:230:TYR:HA	1.67	0.58
2:B:14:GLN:HE21	2:B:149:SER:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ASP:OD1	2:D:85:SER:HB2	2.03	0.58
2:H:67:ASN:HB3	2:H:69:TYR:HE2	1.69	0.58
1:A:224:LYS:HE2	1:A:228:GLU:OE2	2.03	0.58
1:E:160:PRO:HB3	1:E:250:PHE:CE1	2.37	0.58
2:F:70:TYR:CD1	2:F:75:LYS:HE3	2.38	0.58
1:C:207:GLN:HG3	1:C:214:TYR:CZ	2.39	0.58
1:C:183:ARG:NH1	1:C:204:VAL:HG21	2.18	0.58
1:A:182:PRO:O	1:A:239:HIS:HE1	1.87	0.58
1:E:153:ALA:HB2	1:E:241:GLY:HA3	1.86	0.58
2:D:75:LYS:HE3	2:D:76:GLY:N	2.19	0.58
2:D:155:PRO:HD2	2:D:241:THR:HG21	1.86	0.57
1:E:154:PRO:CG	1:E:177:LEU:HD12	2.34	0.57
2:F:194:ALA:HB2	2:H:20:ARG:HG2	1.85	0.57
1:E:149:ARG:HD3	1:E:150:THR:O	2.05	0.57
1:A:179:ASN:HA	1:A:214:TYR:O	2.05	0.57
2:D:93:MET:HB3	2:D:96:LEU:HD21	1.87	0.56
1:A:227:TYR:CZ	1:A:252:ARG:HG3	2.39	0.56
2:F:67:ASN:HB3	2:F:69:TYR:HE2	1.69	0.56
2:F:232:CYS:SG	2:F:245:LYS:HB3	2.46	0.56
1:C:141:GLN:H	1:C:141:GLN:NE2	2.03	0.56
1:C:24:ARG:HD2	1:C:88:ASP:OD1	2.05	0.56
2:D:155:PRO:HB3	2:D:181:TYR:HB3	1.88	0.56
1:E:204:VAL:HG22	1:E:216:LEU:HD12	1.88	0.56
2:B:59:TRP:CG	2:B:67:ASN:HB2	2.41	0.56
2:H:246:LYS:HD3	2:H:248:GLU:OE2	2.06	0.55
1:A:239:HIS:HD2	1:A:241:GLY:H	1.52	0.55
1:A:204:VAL:HG23	1:A:216:LEU:HD12	1.88	0.55
2:D:18:SER:HA	2:D:93:MET:O	2.07	0.55
1:E:227:TYR:CZ	1:E:252:ARG:HG3	2.42	0.55
2:H:67:ASN:HB3	2:H:69:TYR:CE2	2.42	0.55
1:C:227:TYR:OH	1:C:252:ARG:HG3	2.07	0.55
1:G:150:THR:HG22	1:G:151:VAL:O	2.07	0.54
1:C:154:PRO:HB3	1:C:180:PHE:HB3	1.88	0.54
1:G:156:VAL:HG12	1:G:248:LYS:HG3	1.88	0.54
2:H:191:ASN:ND2	2:H:231:ILE:H	2.05	0.54
1:E:150:THR:HG22	1:E:151:VAL:O	2.08	0.54
1:E:156:VAL:HG22	1:E:177:LEU:CD1	2.36	0.54
1:C:153:ALA:HB2	1:C:241:GLY:O	2.07	0.53
1:E:70:ARG:HG2	1:E:74:VAL:HB	1.89	0.53
2:B:186:VAL:HG11	2:B:214:LEU:HD22	1.89	0.53
2:D:221:PRO:O	2:D:224:SER:OG	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:PRO:HG2	2:B:249:PRO:HA	1.89	0.53
2:B:236:HIS:HB3	2:B:241:THR:HB	1.89	0.53
1:C:151:VAL:CG1	1:C:240:GLN:HG2	2.38	0.53
2:F:13:VAL:CG2	2:F:19:LEU:HD22	2.38	0.53
1:A:226:ASP:HA	1:A:229:LYS:HE2	1.90	0.53
1:A:24:ARG:HA	1:A:87:THR:O	2.08	0.53
1:A:2:ILE:HG12	1:A:27:GLN:CG	2.36	0.52
1:A:204:VAL:CG2	1:A:216:LEU:HD12	2.39	0.52
2:F:179:LYS:HG3	2:F:213:SER:OG	2.10	0.52
1:E:186:LYS:HB3	1:E:238:THR:HB	1.92	0.52
2:H:54:TRP:HZ2	2:H:57:SER:HG	1.57	0.52
1:C:229:LYS:HG2	1:C:230:HIS:CE1	2.44	0.52
1:A:227:TYR:CE2	1:A:252:ARG:HG3	2.45	0.52
1:G:101:PHE:CG	1:G:147:ILE:HG13	2.43	0.52
1:E:229:LYS:HE2	1:E:230:HIS:CE1	2.45	0.52
2:B:178:VAL:HB	2:B:214:LEU:CD2	2.40	0.52
2:B:191:ASN:N	2:B:191:ASN:HD22	2.08	0.51
2:B:229:THR:HG23	2:B:246:LYS:CE	2.35	0.51
1:E:70:ARG:CZ	1:E:76:ALA:HA	2.40	0.51
1:A:52:PRO:HG2	2:B:139:TRP:CZ3	2.46	0.51
1:E:152:ALA:O	1:E:180:PHE:HA	2.11	0.50
1:G:14:SER:O	1:G:17:GLU:HB2	2.12	0.50
2:F:194:ALA:HB2	2:H:20:ARG:CG	2.41	0.50
1:A:149:ARG:HD3	1:A:150:THR:O	2.11	0.50
1:G:70:ARG:HD2	1:G:75:PRO:O	2.11	0.50
2:B:222:SER:O	2:B:225:LEU:HG	2.12	0.50
1:E:52:PRO:HG2	2:F:139:TRP:CZ3	2.46	0.50
1:G:146:GLU:HG2	1:G:207:GLN:OE1	2.12	0.50
1:E:183:ARG:CZ	1:E:204:VAL:HG21	2.42	0.50
2:H:13:VAL:HG13	2:H:17:GLY:HA3	1.94	0.50
2:F:10:GLY:HA2	2:F:145:VAL:HG12	1.94	0.49
1:E:208:ASP:OD2	1:E:210:LYS:HE2	2.13	0.49
1:E:58:ASP:OD2	2:F:112:GLY:O	2.30	0.49
2:F:42:HIS:NE2	2:F:57:SER:HB3	2.28	0.49
2:F:58:ILE:HD11	2:F:65:GLY:HA2	1.95	0.49
2:F:178:VAL:HB	2:F:214:LEU:HD22	1.93	0.49
2:B:19:LEU:HD12	3:D:2042:HOH:O	2.13	0.49
1:E:178:ASN:OD1	1:E:179:ASN:OD1	2.30	0.48
2:H:233:ASN:HB3	2:H:242:LYS:NZ	2.28	0.48
2:B:83:ASP:CG	2:B:86:LYS:HD2	2.33	0.48
1:C:211:ASP:O	1:C:212:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ARG:HG2	1:C:74:VAL:HB	1.94	0.48
2:H:246:LYS:HD3	2:H:248:GLU:CD	2.34	0.48
1:A:58:ASP:O	1:A:67:SER:HB3	2.13	0.48
1:C:251:ASN:HD22	1:C:251:ASN:N	2.10	0.48
1:G:146:GLU:OE2	1:G:181:TYR:HE2	1.96	0.48
2:H:43:TRP:NE1	2:H:91:LEU:HB2	2.29	0.48
1:C:210:LYS:HB3	1:C:210:LYS:HE2	1.60	0.48
2:F:221:PRO:O	2:F:224:SER:OG	2.30	0.48
2:H:191:ASN:HD21	2:H:231:ILE:H	1.62	0.47
1:A:179:ASN:HB3	1:A:213:THR:OG1	2.14	0.47
1:A:200:SER:HA	1:A:219:THR:O	2.13	0.47
2:H:82:ARG:HE	2:H:84:ASN:ND2	2.11	0.47
2:D:180:ASP:HB3	2:D:211:LEU:HD13	1.97	0.47
1:G:181:TYR:CG	1:G:182:PRO:HA	2.48	0.47
1:A:137:PRO:HG2	2:B:54:TRP:CD2	2.50	0.47
2:F:13:VAL:CG1	2:F:17:GLY:HA3	2.45	0.47
2:D:42:HIS:CD2	2:D:57:SER:HB3	2.49	0.47
1:A:153:ALA:HB1	1:A:242:LEU:CD2	2.45	0.47
1:A:160:PRO:HB3	1:A:250:PHE:CE1	2.50	0.47
1:G:227:TYR:O	1:G:233:TYR:OH	2.32	0.47
1:E:211:ASP:O	1:E:212:SER:HB2	2.15	0.46
1:A:188:GLN:HB2	1:A:236:GLU:HB3	1.96	0.46
1:C:181:TYR:CG	1:C:182:PRO:HA	2.50	0.46
1:G:211:ASP:O	1:G:212:SER:HB2	2.15	0.46
2:B:65:GLY:O	2:B:67:ASN:OD1	2.34	0.46
2:F:153:LYS:HG2	2:F:154:GLY:O	2.16	0.46
1:C:77:ARG:HD3	3:C:2023:HOH:O	2.15	0.46
2:B:175:GLY:HA2	2:B:190:TRP:CH2	2.51	0.46
2:B:189:SER:OG	2:B:233:ASN:OD1	2.30	0.46
1:C:178:ASN:HD21	2:D:200:HIS:HD2	1.64	0.46
2:H:162:PRO:HG2	2:H:249:PRO:CA	2.39	0.46
2:H:72:ASP:HA	2:H:75:LYS:NZ	2.30	0.46
2:F:78:PHE:CZ	2:F:93:MET:HE2	2.51	0.46
1:A:177:LEU:HD11	1:A:187:VAL:CG2	2.46	0.46
1:E:177:LEU:HD11	1:E:237:VAL:CG2	2.41	0.46
2:F:190:TRP:CH2	2:F:232:CYS:HB3	2.51	0.46
2:B:155:PRO:HD2	2:B:241:THR:HG21	1.97	0.45
1:E:154:PRO:HA	1:E:178:ASN:O	2.16	0.45
2:F:158:PHE:HB2	2:F:177:LEU:HB3	1.98	0.45
1:C:227:TYR:CE2	1:C:252:ARG:HD3	2.51	0.45
2:H:13:VAL:CG1	2:H:17:GLY:HA3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:TYR:OH	1:E:252:ARG:HG3	2.16	0.45
2:H:29:PHE:CE2	2:H:31:PHE:HA	2.52	0.45
2:B:30:THR:HG22	2:B:32:ARG:HG3	1.99	0.45
1:E:24:ARG:NH2	1:E:87:THR:OG1	2.50	0.45
2:B:6:GLU:HG3	2:B:106:CYS:SG	2.56	0.45
1:E:190:LYS:HE2	3:E:2045:HOH:O	2.17	0.45
1:G:228:GLU:O	1:G:252:ARG:NH2	2.50	0.45
2:B:19:LEU:HD11	3:B:2003:HOH:O	2.16	0.45
1:C:228:GLU:O	1:C:252:ARG:NH2	2.50	0.45
1:E:18:ARG:NH2	3:E:2006:HOH:O	2.50	0.45
2:D:32:ARG:HA	2:D:84:ASN:ND2	2.32	0.45
1:E:8:PRO:CG	1:E:11:LEU:HD13	2.47	0.45
1:G:146:GLU:HG2	1:G:147:ILE:N	2.33	0.44
1:G:178:ASN:OD1	1:G:179:ASN:OD1	2.35	0.44
2:B:75:LYS:HE3	2:B:75:LYS:HB2	1.76	0.44
1:G:137:PRO:HD2	2:H:54:TRP:CD2	2.52	0.44
2:H:159:PRO:HD3	2:H:245:LYS:HE3	1.99	0.44
2:H:41:MET:HB3	2:H:89:LEU:HD22	1.99	0.44
1:A:50:GLN:NE2	3:A:2014:HOH:O	2.50	0.44
2:F:23:CYS:HB3	2:F:89:LEU:HB3	1.98	0.44
1:G:101:PHE:CD1	1:G:145:VAL:HG12	2.52	0.44
1:C:24:ARG:NH1	1:C:88:ASP:OD1	2.50	0.44
1:C:164:GLU:CA	1:C:167:LYS:HD3	2.41	0.44
1:C:227:TYR:O	1:C:233:TYR:OH	2.30	0.44
1:E:208:ASP:OD1	1:E:210:LYS:HD3	2.17	0.44
1:G:11:LEU:HG	1:G:13:LEU:HD11	1.98	0.44
2:H:72:ASP:CG	2:H:75:LYS:HZ1	2.21	0.44
1:A:58:ASP:OD2	2:B:112:GLY:O	2.35	0.44
1:C:252:ARG:HD2	1:C:252:ARG:HH11	1.57	0.44
1:G:208:ASP:OD2	1:G:210:LYS:HE2	2.17	0.44
1:G:24:ARG:HG2	1:G:87:THR:O	2.18	0.44
2:H:48:PRO:O	2:H:50:LYS:HD3	2.17	0.44
1:C:178:ASN:HD21	2:D:200:HIS:CD2	2.35	0.44
1:E:177:LEU:CD1	1:E:237:VAL:HG11	2.47	0.44
2:B:71:ALA:O	2:B:74:VAL:HG22	2.17	0.44
1:C:226:ASP:HA	1:C:229:LYS:CE	2.47	0.44
2:F:2:VAL:N	3:F:2001:HOH:O	2.50	0.44
2:H:101:THR:HG23	2:H:146:THR:HA	2.00	0.44
1:E:181:TYR:CG	1:E:182:PRO:HA	2.53	0.43
1:E:227:TYR:CE2	1:E:252:ARG:HD3	2.53	0.43
2:F:75:LYS:HE2	2:F:75:LYS:CA	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:PRO:HD2	2:H:241:THR:CG2	2.46	0.43
2:H:233:ASN:HB3	2:H:242:LYS:HZ3	1.83	0.43
2:F:237:LYS:HB2	2:F:238:PRO:HD3	1.99	0.43
1:E:52:PRO:HD2	2:F:139:TRP:CE3	2.53	0.43
2:F:19:LEU:HD23	2:F:145:VAL:CG1	2.48	0.43
2:H:6:GLU:CD	2:H:142:GLY:H	2.19	0.43
2:H:82:ARG:NE	2:H:84:ASN:HD21	2.15	0.43
1:E:56:ILE:HD13	1:E:70:ARG:HA	2.01	0.43
2:F:236:HIS:CE1	2:F:238:PRO:HB2	2.53	0.43
1:G:156:VAL:CG1	1:G:248:LYS:HG3	2.48	0.43
2:H:2:VAL:HA	2:H:27:GLY:HA3	1.99	0.43
1:A:181:TYR:CG	1:A:182:PRO:HA	2.53	0.43
2:D:236:HIS:HB3	2:D:241:THR:HB	1.99	0.43
1:G:39:ASN:O	1:G:58:ASP:HA	2.18	0.43
2:H:191:ASN:ND2	3:H:2049:HOH:O	2.50	0.43
1:E:12:SER:OG	1:E:146:GLU:OE2	2.30	0.43
2:B:59:TRP:CD2	2:B:67:ASN:HB2	2.53	0.43
2:B:83:ASP:OD2	2:B:85:SER:OG	2.30	0.43
2:B:190:TRP:CH2	2:B:232:CYS:HB3	2.54	0.43
1:E:155:SER:HB2	1:E:157:PHE:CE2	2.53	0.42
1:C:239:HIS:HB3	1:C:242:LEU:HD12	2.00	0.42
2:H:172:ALA:CB	2:H:225:LEU:HD11	2.49	0.42
2:H:32:ARG:O	2:H:60:TYR:HB2	2.19	0.42
1:G:237:VAL:O	1:G:245:PRO:HA	2.19	0.42
1:G:208:ASP:OD2	1:G:210:LYS:HG3	2.19	0.42
2:D:6:GLU:OE1	2:D:6:GLU:N	2.49	0.42
1:E:3:VAL:HB	1:E:26:SER:HB3	2.01	0.42
2:F:162:PRO:HD3	2:F:174:LEU:CB	2.50	0.42
1:E:21:LEU:N	1:E:21:LEU:HD12	2.33	0.42
1:A:210:LYS:HB2	1:A:210:LYS:HE3	1.77	0.42
1:E:204:VAL:HG12	1:E:205:THR:O	2.20	0.42
1:A:190:LYS:NZ	1:A:236:GLU:OE2	2.50	0.41
1:C:202:GLU:HA	1:C:217:SER:O	2.20	0.41
1:C:44:TYR:OH	1:C:107:HIS:HD2	2.04	0.41
2:B:188:VAL:HA	2:B:233:ASN:O	2.21	0.41
2:H:199:VAL:HG22	2:H:218:VAL:HG22	2.02	0.41
2:D:14:GLN:HE21	2:D:15:PRO:HD2	1.86	0.41
2:F:13:VAL:HG12	2:F:17:GLY:HA3	2.03	0.41
1:C:161:PRO:HD3	1:C:173:VAL:HG22	2.01	0.41
1:E:170:THR:HG22	1:E:171:ALA:N	2.35	0.41
2:F:41:MET:HB3	2:F:89:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:TRP:HE3	2:D:60:TYR:CE1	2.39	0.41
1:E:154:PRO:HG3	1:E:177:LEU:HD12	2.01	0.41
1:E:252:ARG:HD2	1:E:252:ARG:HH11	1.45	0.41
2:F:39:SER:HB3	2:F:108:ARG:HG2	2.03	0.41
1:E:154:PRO:HG2	1:E:177:LEU:HD12	2.03	0.41
1:E:24:ARG:HH21	1:E:88:ASP:HB2	1.83	0.41
2:F:10:GLY:HA2	2:F:145:VAL:CG1	2.51	0.41
2:B:186:VAL:HG11	2:B:214:LEU:CD2	2.50	0.41
1:A:107:HIS:HE1	3:B:2031:HOH:O	2.02	0.41
1:A:208:ASP:OD2	1:A:210:LYS:HG3	2.20	0.41
1:C:160:PRO:HB3	1:C:250:PHE:CZ	2.56	0.41
1:C:181:TYR:CD2	1:C:182:PRO:HA	2.56	0.40
2:H:237:LYS:HB2	2:H:238:PRO:HD3	2.04	0.40
2:D:11:GLY:N	2:D:144:LEU:O	2.55	0.40
1:G:43:TRP:CE2	1:G:91:LEU:HB2	2.56	0.40
2:H:181:TYR:OH	2:H:204:ALA:HB2	2.22	0.40
2:D:31:PHE:CD2	2:D:87:ASN:HA	2.57	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	211/215 (98%)	206 (98%)	5 (2%)	0	100 100
1	C	210/215 (98%)	203 (97%)	7 (3%)	0	100 100
1	E	211/215 (98%)	205 (97%)	6 (3%)	0	100 100
1	G	210/215 (98%)	206 (98%)	4 (2%)	0	100 100
2	B	210/229 (92%)	201 (96%)	8 (4%)	1 (0%)	29 18
2	D	209/229 (91%)	200 (96%)	7 (3%)	2 (1%)	15 6
2	F	208/229 (91%)	200 (96%)	7 (3%)	1 (0%)	29 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	207/229 (90%)	200 (97%)	6 (3%)	1 (0%)	29 18
All	All	1676/1776 (94%)	1621 (97%)	50 (3%)	5 (0%)	41 31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	134	GLY
2	D	10	GLY
2	H	134	GLY
2	D	134	GLY
2	B	65	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	186/187 (100%)	166 (89%)	20 (11%)	6 2
1	C	186/187 (100%)	169 (91%)	17 (9%)	9 3
1	E	186/187 (100%)	171 (92%)	15 (8%)	11 4
1	G	186/187 (100%)	172 (92%)	14 (8%)	13 5
2	B	175/190 (92%)	164 (94%)	11 (6%)	18 8
2	D	174/190 (92%)	155 (89%)	19 (11%)	6 2
2	F	173/190 (91%)	153 (88%)	20 (12%)	5 1
2	H	173/190 (91%)	157 (91%)	16 (9%)	9 3
All	All	1439/1508 (95%)	1307 (91%)	132 (9%)	9 3

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	24	ARG
1	A	27	GLN

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	53	ARG
1	A	88	ASP
1	A	90	THR
1	A	146	GLU
1	A	148	LYS
1	A	149	ARG
1	A	155	SER
1	A	177	LEU
1	A	179	ASN
1	A	183	ARG
1	A	197	SER
1	A	204	VAL
1	A	210	LYS
1	A	229	LYS
1	A	231	LYS
1	A	244	SER
2	B	12	LEU
2	B	14	GLN
2	B	50	LYS
2	B	191	ASN
2	B	214	LEU
2	B	222	SER
2	B	224	SER
2	B	227	THR
2	B	233	ASN
2	B	242	LYS
2	B	243	VAL
1	C	11	LEU
1	C	27	GLN
1	C	30	SER
1	C	41	LEU
1	C	67	SER
1	C	88	ASP
1	C	90	THR
1	C	141	GLN
1	C	146	GLU
1	C	149	ARG
1	C	155	SER
1	C	183	ARG
1	C	210	LYS
1	C	229	LYS

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Mol	Chain	Res	Type
1	C	240	GLN
1	C	244	SER
1	C	251	ASN
2	D	3	GLN
2	D	12	LEU
2	D	14	GLN
2	D	18	SER
2	D	22	SER
2	D	30	THR
2	D	33	ASN
2	D	57	SER
2	D	75	LYS
2	D	144	LEU
2	D	214	LEU
2	D	222	SER
2	D	224	SER
2	D	227	THR
2	D	233	ASN
2	D	237	LYS
2	D	242	LYS
2	D	245	LYS
2	D	248	GLU
1	E	7	SER
1	E	18	ARG
1	E	24	ARG
1	E	41	LEU
1	E	50	GLN
1	E	88	ASP
1	E	149	ARG
1	E	155	SER
1	E	164	GLU
1	E	186	LYS
1	E	210	LYS
1	E	231	LYS
1	E	238	THR
1	E	244	SER
1	E	252	ARG
2	F	3	GLN
2	F	8	SER
2	F	12	LEU
2	F	19	LEU
2	F	30	THR

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Mol	Chain	Res	Type
2	F	32	ARG
2	F	50	LYS
2	F	57	SER
2	F	75	LYS
2	F	86	LYS
2	F	95	SER
2	F	144	LEU
2	F	151	SER
2	F	174	LEU
2	F	214	LEU
2	F	224	SER
2	F	227	THR
2	F	240	ASN
2	F	242	LYS
2	F	245	LYS
1	G	1	ASP
1	G	24	ARG
1	G	41	LEU
1	G	69	SER
1	G	88	ASP
1	G	135	ILE
1	G	141	GLN
1	G	149	ARG
1	G	155	SER
1	G	167	LYS
1	G	183	ARG
1	G	231	LYS
1	G	244	SER
1	G	252	ARG
2	H	12	LEU
2	H	20	ARG
2	H	32	ARG
2	H	57	SER
2	H	60	TYR
2	H	75	LYS
2	H	141	GLN
2	H	144	LEU
2	H	213	SER
2	H	214	LEU
2	H	227	THR
2	H	228	GLN
2	H	233	ASN

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Mol	Chain	Res	Type
2	H	240	ASN
2	H	242	LYS
2	H	248	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	107	HIS
1	A	178	ASN
1	A	193	ASN
1	A	201	GLN
1	A	230	HIS
1	A	239	HIS
1	A	240	GLN
1	A	251	ASN
2	B	14	GLN
2	B	33	ASN
2	B	92	GLN
2	B	191	ASN
1	C	50	GLN
1	C	107	HIS
1	C	141	GLN
1	C	201	GLN
1	C	230	HIS
1	C	251	ASN
2	D	14	GLN
2	D	33	ASN
2	D	84	ASN
2	D	191	ASN
2	D	200	HIS
1	E	107	HIS
1	E	179	ASN
1	E	188	GLN
1	E	193	ASN
1	E	251	ASN
2	F	33	ASN
2	F	84	ASN
2	F	191	ASN
2	F	228	GLN
1	G	107	HIS
1	G	193	ASN

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Mol	Chain	Res	Type
1	G	251	ASN
2	H	84	ASN
2	H	191	ASN
2	H	228	GLN

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	213/215 (99%)	-0.15	0 100 100	13, 21, 34, 51	0
1	C	212/215 (98%)	-0.22	0 100 100	13, 21, 33, 51	0
1	E	213/215 (99%)	-0.15	1 (0%) 91 92	14, 22, 34, 51	0
1	G	212/215 (98%)	-0.21	2 (0%) 84 85	13, 21, 33, 51	0
2	B	214/229 (93%)	0.03	1 (0%) 91 92	14, 24, 45, 60	0
2	D	213/229 (93%)	0.14	9 (4%) 36 39	15, 24, 46, 59	0
2	F	212/229 (92%)	0.08	5 (2%) 59 62	16, 24, 44, 60	0
2	H	211/229 (92%)	-0.02	5 (2%) 59 62	15, 24, 43, 60	0
All	All	1700/1776 (95%)	-0.06	23 (1%) 75 77	13, 23, 40, 60	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	169	GLY	7.4
2	F	169	GLY	3.5
2	H	225	LEU	3.2
2	H	227	THR	3.1
2	F	65	GLY	3.0
2	H	226	GLY	2.8
2	H	60	TYR	2.8
2	D	59	TRP	2.7
2	F	249	PRO	2.7
2	D	64	SER	2.5
2	D	1	GLN	2.4
1	G	210	LYS	2.3
2	D	32	ARG	2.3
1	G	1	ASP	2.3
2	F	13	VAL	2.3
2	D	170	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	64	SER	2.2
2	H	170	GLY	2.2
2	D	60	TYR	2.2
2	D	226	GLY	2.2
1	E	253	GLY	2.2
2	B	64	SER	2.2
2	D	66	SER	2.1

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.