Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 05:37 PM EDT

PDB ID	:	7RCO
Title	:	Crystal structure of human TGF-beta-2 bound to 4A11.V2 Fab
Authors	:	Yin, J.; Lupardus, P.J.; Sudhamsu, J.
Deposited on	:	2021-07-07
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

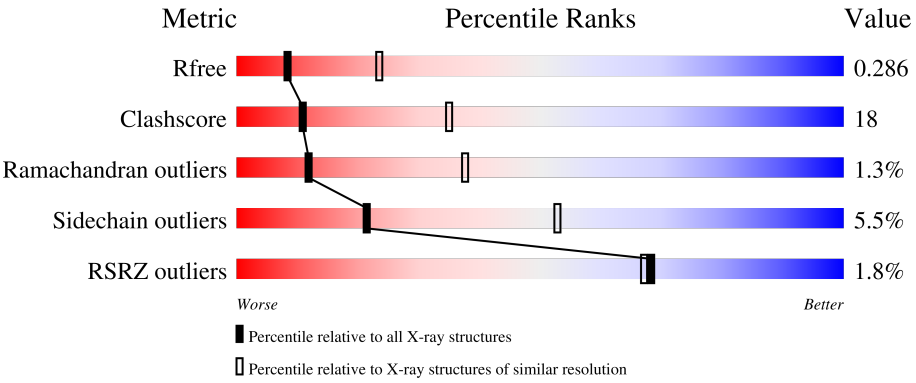
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	112	3% 65% 31%
1	B	112	65% 33%
2	C	219	77% 21%
2	E	219	5% 58% 32% 7%
3	D	233	% 60% 30% 7%

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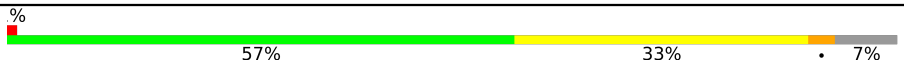
Mol	Chain	Length	Quality of chain
3	F	233	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8200 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 Transforming growth factor beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			882	560	148	164	10			
1	B	112	Total	C	N	O	S	0	0	0
			890	566	149	165	10			

- Molecule 2 is a protein called 4A11.V2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1643	1027	273	339	4			
2	E	204	Total	C	N	O	S	0	0	0
			1547	968	255	320	4			

- Molecule 3 is a protein called 4A11.V2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	216	Total	C	N	O	S	0	0	0
			1595	1013	267	308	7			
3	F	216	Total	C	N	O	S	0	0	0
			1595	1013	267	308	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	8	Total	O	0	0
			8	8		
4	C	6	Total	O	0	0
			6	6		
4	D	10	Total	O	0	0
			10	10		

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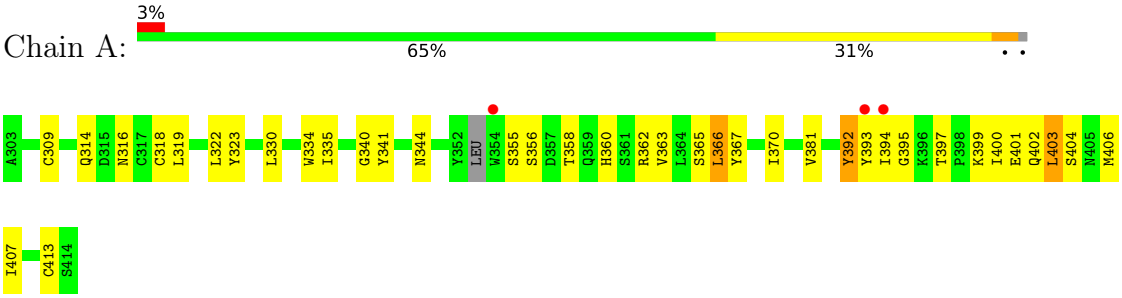
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	10	Total O 10 10	0	0
4	F	9	Total O 9 9	0	0

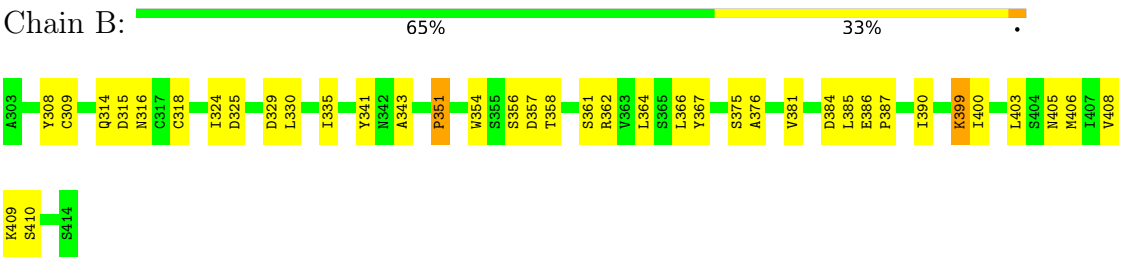
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

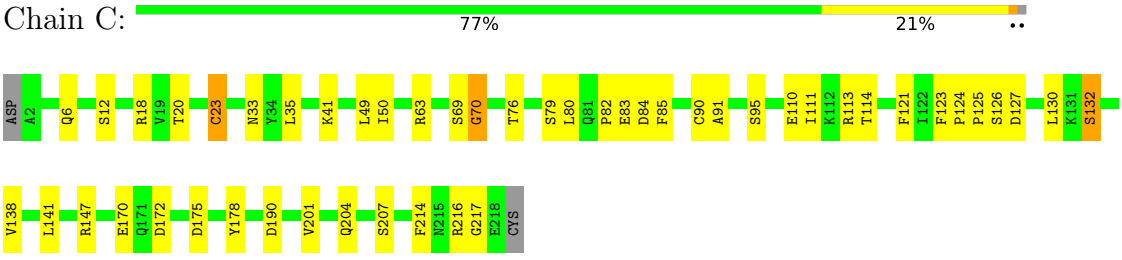
• Molecule 1: Transforming growth factor beta-2



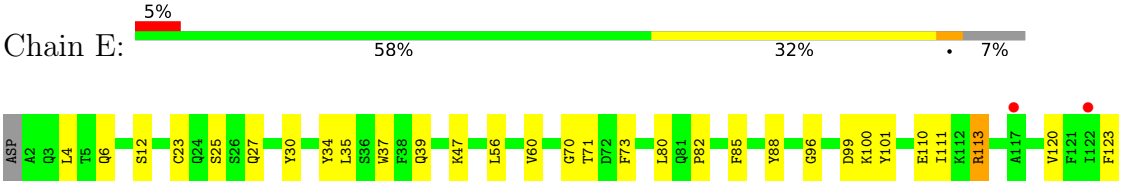
• Molecule 1: Transforming growth factor beta-2

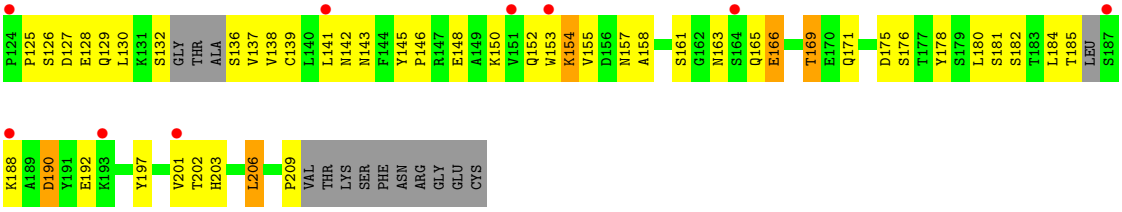


• Molecule 2: 4A11.V2 Fab Light Chain

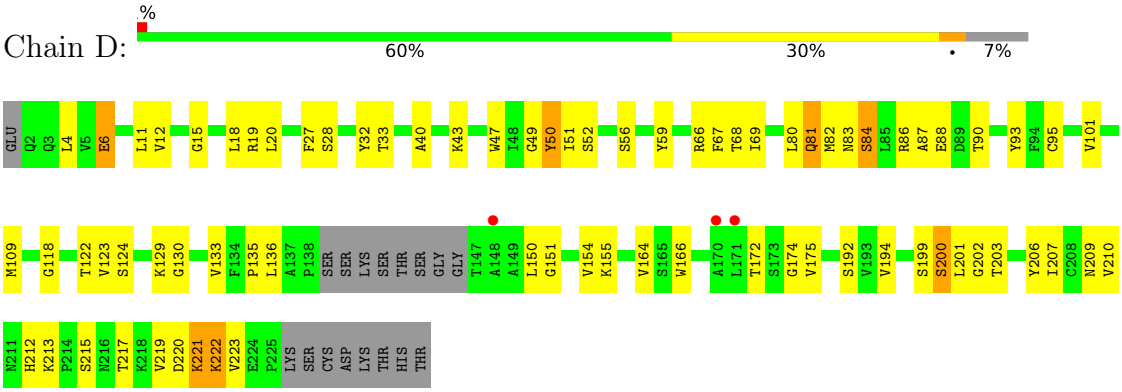


• Molecule 2: 4A11.V2 Fab Light Chain

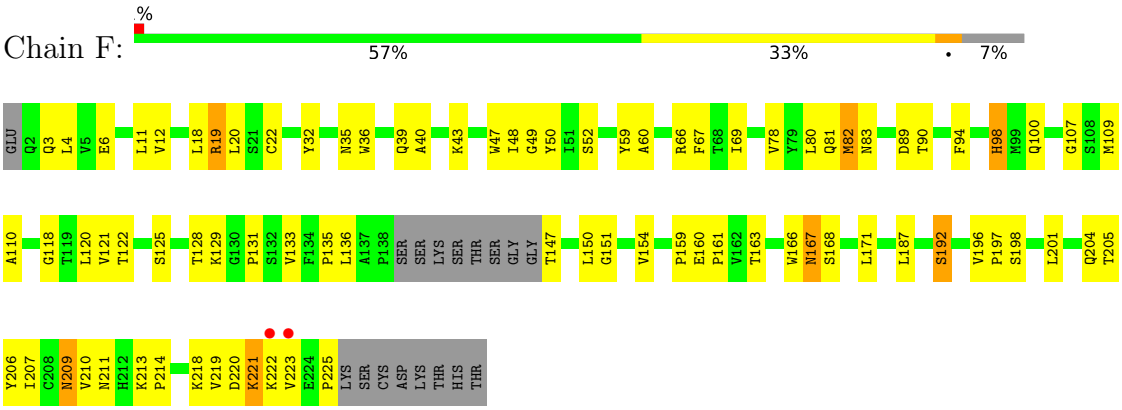




• Molecule 3: 4A11.V2 Fab Heavy Chain



• Molecule 3: 4A11.V2 Fab Heavy Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.15Å 103.48Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 2.90 45.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.95-2.90) 98.6 (45.95-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.208 , 0.286 0.211 , 0.286	Depositor DCC
R_{free} test set	1335 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8200	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.68	0/905	0.67	0/1228
1	B	0.55	0/914	0.64	0/1242
2	C	0.53	0/1679	0.64	0/2279
2	E	0.56	0/1580	0.68	0/2143
3	D	0.64	0/1637	0.70	0/2234
3	F	0.49	0/1637	0.67	0/2234
All	All	0.57	0/8352	0.67	0/11360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	882	0	846	30	0
1	B	890	0	858	31	0
2	C	1643	0	1583	32	0
2	E	1547	0	1484	82	0
3	D	1595	0	1555	64	0
3	F	1595	0	1555	73	0
4	A	5	0	0	0	0
4	B	8	0	0	0	0
4	C	6	0	0	2	0
4	D	10	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	10	0	0	0	0
4	F	9	0	0	4	0
All	All	8200	0	7881	289	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 18.

All (289) 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:367:TYR:CD2	1:B:324:ILE:HD13	1.96	0.99
2:E:203:HIS:H	2:E:206:LEU:HD11	1.30	0.97
3:D:133:VAL:HG21	3:D:219:VAL:HG11	1.43	0.97
3:F:133:VAL:HG21	3:F:210:VAL:HG11	1.50	0.94
2:C:20:THR:HG22	2:C:76:THR:HG23	1.54	0.89
3:D:90:THR:HG23	3:D:123:VAL:HG22	1.56	0.88
3:D:207:ILE:HB	3:D:221:LYS:O	1.74	0.86
3:F:168:SER:H	3:F:209:ASN:HD21	1.20	0.86
3:D:86:ARG:O	3:D:123:VAL:HG21	1.76	0.85
2:E:130:LEU:HB3	2:E:188:LYS:HZ1	1.42	0.84
3:F:35:ASN:HD21	3:F:98:HIS:CE1	1.96	0.83
3:D:212:HIS:HB3	3:D:217:THR:OG1	1.78	0.82
1:A:356:SER:HB3	1:A:362:ARG:HG2	1.59	0.82
3:D:215:SER:OG	3:D:217:THR:HG23	1.81	0.80
3:D:90:THR:HG22	3:D:122:THR:HA	1.63	0.79
1:A:367:TYR:CD2	1:B:324:ILE:CD1	2.68	0.77
2:E:203:HIS:N	2:E:206:LEU:HD11	2.00	0.77
2:E:130:LEU:HB3	2:E:188:LYS:NZ	2.01	0.76
2:E:82:PRO:HA	2:E:111:ILE:HD13	1.68	0.75
3:F:90:THR:HG23	3:F:122:THR:HA	1.69	0.74
2:E:96:GLY:O	2:E:100:LYS:HE2	1.86	0.74
2:E:188:LYS:HG2	2:E:192:GLU:CD	2.07	0.73
2:C:113:ARG:NH1	2:C:114:THR:O	2.20	0.73
2:C:141:LEU:HD11	2:C:201:VAL:HG21	1.71	0.73
3:F:19:ARG:HB2	3:F:81:GLN:NE2	2.04	0.73
2:C:216:ARG:HG2	4:C:301:HOH:O	1.88	0.72
1:A:330:LEU:HD23	1:B:366:LEU:HB3	1.71	0.72
1:B:314:GLN:NE2	1:B:316:ASN:HB2	2.06	0.71
2:E:188:LYS:HG2	2:E:192:GLU:OE1	1.90	0.70
2:C:63:ARG:NH2	2:C:84:ASP:OD2	2.26	0.69
2:E:188:LYS:HE3	2:E:192:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:129:LYS:HD2	3:F:187:LEU:HD21	1.76	0.67
3:D:210:VAL:HG12	3:D:219:VAL:HB	1.76	0.67
3:F:167:ASN:HA	3:F:207:ILE:HG23	1.77	0.67
3:D:129:LYS:HD3	3:D:130:GLY:O	1.93	0.67
3:D:12:VAL:O	3:D:123:VAL:HA	1.97	0.65
2:C:49:LEU:CB	2:C:50:ILE:HD12	2.27	0.65
2:E:154:LYS:NZ	2:E:157:ASN:HA	2.12	0.65
2:E:35:LEU:HD13	2:E:73:PHE:CD1	2.32	0.64
1:A:319:LEU:HD21	1:A:344:ASN:HD22	1.63	0.64
3:D:164:VAL:HG22	3:D:210:VAL:HG23	1.78	0.64
2:E:203:HIS:HB3	2:E:206:LEU:HG	1.79	0.64
2:C:126:SER:O	2:C:130:LEU:HG	1.98	0.63
3:D:207:ILE:HD13	3:D:220:ASP:HB3	1.79	0.63
2:E:206:LEU:HD12	2:E:206:LEU:O	1.99	0.63
3:F:168:SER:N	3:F:209:ASN:HD21	1.93	0.63
1:A:314:GLN:HG3	1:A:316:ASN:H	1.64	0.62
2:C:49:LEU:HB2	2:C:50:ILE:HD12	1.82	0.62
3:F:147:THR:N	3:F:198:SER:HB2	2.14	0.62
2:C:12:SER:HA	2:C:110:GLU:O	2.00	0.61
2:E:163:ASN:HD21	2:E:185:THR:H	1.45	0.61
3:F:196:VAL:HG21	3:F:206:TYR:CZ	2.36	0.61
1:B:335:ILE:HG12	1:B:390:ILE:HD13	1.83	0.61
3:F:120:LEU:HD12	3:F:121:VAL:H	1.65	0.60
2:E:4:LEU:HD12	2:E:23:CYS:SG	2.40	0.60
2:E:34:TYR:OH	3:F:107:GLY:HA3	2.02	0.60
1:A:366:LEU:HD22	1:A:370:ILE:HD12	1.84	0.60
2:C:141:LEU:HD11	2:C:201:VAL:CG2	2.32	0.59
3:D:150:LEU:HD13	3:D:223:VAL:HG21	1.84	0.59
3:D:206:TYR:O	3:D:223:VAL:HG22	2.03	0.59
3:F:167:ASN:N	3:F:207:ILE:O	2.29	0.59
2:C:80:LEU:HD21	2:C:111:ILE:CD1	2.32	0.59
1:A:381:VAL:HG11	1:B:381:VAL:HG11	1.85	0.59
3:D:154:VAL:HG21	3:D:210:VAL:HG21	1.84	0.59
2:E:56:LEU:HD21	2:E:60:VAL:O	2.03	0.58
2:E:142:ASN:OD1	2:E:143:ASN:ND2	2.36	0.58
3:D:215:SER:OG	3:D:217:THR:CG2	2.51	0.58
3:F:47:TRP:CZ2	3:F:49:GLY:HA2	2.38	0.58
2:E:6:GLN:NE2	2:E:88:TYR:O	2.35	0.58
1:A:397:THR:O	1:A:399:LYS:NZ	2.35	0.57
3:D:90:THR:CG2	3:D:123:VAL:H	2.17	0.57
2:E:129:GLN:OE1	2:E:136:SER:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:PRO:HD3	2:E:137:VAL:HG12	1.85	0.57
2:E:137:VAL:HG22	2:E:184:LEU:HD23	1.86	0.57
2:E:99:ASP:OD1	3:F:60:ALA:HA	2.04	0.57
2:E:154:LYS:NZ	2:E:157:ASN:OD1	2.36	0.57
3:F:163:THR:OG1	3:F:211:ASN:HB3	2.04	0.57
2:E:150:LYS:HB3	2:E:202:THR:OG1	2.05	0.57
2:E:169:THR:HG21	2:E:178:TYR:HA	1.87	0.57
1:A:403:LEU:HB3	1:A:406:MET:HG3	1.87	0.56
1:A:363:VAL:HG13	1:B:330:LEU:HD21	1.87	0.56
2:E:39:GLN:O	2:E:47:LYS:N	2.35	0.56
2:E:154:LYS:NZ	2:E:157:ASN:CA	2.69	0.56
2:E:154:LYS:HZ1	2:E:157:ASN:CA	2.19	0.56
3:D:18:LEU:HD21	3:D:20:LEU:HD23	1.86	0.56
2:E:163:ASN:ND2	2:E:185:THR:H	2.03	0.56
3:D:207:ILE:HG22	3:D:222:LYS:HB2	1.87	0.55
1:A:314:GLN:HG3	1:A:316:ASN:N	2.22	0.55
3:D:86:ARG:NH2	4:D:302:HOH:O	2.36	0.55
2:E:123:PHE:HB2	2:E:138:VAL:HG22	1.89	0.55
3:F:211:ASN:ND2	3:F:218:LYS:HE3	2.21	0.55
3:F:120:LEU:HD12	3:F:121:VAL:N	2.22	0.54
2:E:180:LEU:HD12	2:E:181:SER:H	1.72	0.54
3:F:166:TRP:NE1	3:F:192:SER:OG	2.39	0.54
3:F:201:LEU:HD13	3:F:206:TYR:HD2	1.73	0.54
1:B:314:GLN:HE21	1:B:316:ASN:HB2	1.72	0.54
3:F:59:TYR:HE1	3:F:69:ILE:HG13	1.72	0.54
2:E:139:CYS:HB2	2:E:153:TRP:CH2	2.43	0.53
3:F:12:VAL:HG11	3:F:18:LEU:HD22	1.90	0.53
3:F:204:GLN:OE1	3:F:205:THR:N	2.42	0.53
2:E:146:PRO:HB2	2:E:148:GLU:OE2	2.07	0.53
3:D:33:THR:HG23	3:D:52:SER:HA	1.91	0.53
2:E:139:CYS:HB2	2:E:153:TRP:CZ2	2.44	0.53
2:E:123:PHE:HB2	2:E:138:VAL:CG2	2.39	0.53
2:E:125:PRO:CD	2:E:137:VAL:HG12	2.38	0.53
3:F:196:VAL:HG23	3:F:197:PRO:HD2	1.91	0.53
2:E:113:ARG:HD2	2:E:175:ASP:O	2.09	0.52
3:F:36:TRP:O	3:F:48:ILE:HG12	2.08	0.52
1:A:355:SER:HB2	1:A:413:CYS:H	1.74	0.52
3:D:18:LEU:CD2	3:D:20:LEU:CD2	2.87	0.52
3:D:19:ARG:HD2	3:F:81:GLN:NE2	2.25	0.52
2:E:101:TYR:CE1	3:F:110:ALA:HA	2.44	0.52
3:F:22:CYS:HB3	3:F:78:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:39:GLN:NE2	3:F:43:LYS:O	2.39	0.52
2:E:23:CYS:HB2	2:E:37:TRP:CH2	2.44	0.52
3:D:47:TRP:CZ2	3:D:49:GLY:HA2	2.44	0.52
3:D:87:ALA:HA	3:D:123:VAL:CG2	2.39	0.52
2:E:203:HIS:CA	2:E:206:LEU:HD11	2.40	0.52
2:E:163:ASN:HD21	2:E:185:THR:N	2.08	0.51
3:D:67:PHE:HD1	3:D:82:MET:HG2	1.74	0.51
2:C:80:LEU:HD21	2:C:111:ILE:HD12	1.90	0.51
2:E:130:LEU:HD22	2:E:188:LYS:NZ	2.26	0.51
3:F:100:GLN:NE2	4:F:301:HOH:O	2.30	0.51
2:E:123:PHE:CE1	3:F:150:LEU:HA	2.47	0.50
2:C:6:GLN:HB3	2:C:23:CYS:SG	2.51	0.50
3:D:18:LEU:HD21	3:D:20:LEU:CD2	2.41	0.50
3:D:93:TYR:O	3:D:118:GLY:HA2	2.11	0.50
3:F:66:ARG:NH1	3:F:89:ASP:OD2	2.44	0.50
3:D:66:ARG:HD3	4:D:302:HOH:O	2.11	0.50
2:E:203:HIS:HB3	2:E:206:LEU:CG	2.41	0.50
3:F:131:PRO:HB2	3:F:154:VAL:HG13	1.92	0.50
3:F:196:VAL:HG21	3:F:206:TYR:CE2	2.46	0.50
3:F:210:VAL:CG1	3:F:219:VAL:HB	2.41	0.49
2:C:35:LEU:HA	2:C:91:ALA:O	2.12	0.49
2:C:85:PHE:HZ	2:C:170:GLU:HB3	1.78	0.49
3:D:151:GLY:HA2	3:D:166:TRP:CZ2	2.47	0.49
3:F:201:LEU:HD21	3:F:225:PRO:HD3	1.92	0.49
2:C:110:GLU:OE2	2:C:178:TYR:OH	2.25	0.49
1:B:356:SER:HB2	1:B:362:ARG:NH1	2.28	0.49
2:E:101:TYR:HE1	3:F:110:ALA:HA	1.77	0.49
2:E:154:LYS:HZ1	2:E:157:ASN:CB	2.25	0.49
1:A:360:HIS:CE1	1:B:408:VAL:HG23	2.48	0.49
3:F:19:ARG:NH2	4:F:302:HOH:O	2.35	0.49
3:D:40:ALA:HB3	3:D:43:LYS:HB2	1.95	0.49
3:D:67:PHE:CD1	3:D:82:MET:HG2	2.48	0.48
2:E:12:SER:HA	2:E:110:GLU:O	2.13	0.48
2:C:49:LEU:HB3	2:C:50:ILE:HD12	1.95	0.48
2:C:216:ARG:N	4:C:301:HOH:O	2.28	0.48
3:F:19:ARG:NE	4:F:302:HOH:O	2.34	0.48
2:E:166:GLU:HB2	2:E:180:LEU:HD11	1.95	0.48
2:E:188:LYS:CG	2:E:192:GLU:OE1	2.62	0.48
2:C:113:ARG:HG3	2:C:114:THR:O	2.14	0.48
3:F:150:LEU:HD13	3:F:223:VAL:HG11	1.94	0.48
1:A:366:LEU:HD22	1:A:370:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASP:OD1	2:E:30:TYR:OH	2.22	0.48
2:E:120:VAL:HG13	2:E:141:LEU:HD23	1.95	0.48
2:E:138:VAL:HG21	3:F:136:LEU:HD13	1.95	0.48
3:F:35:ASN:ND2	3:F:98:HIS:CE1	2.74	0.48
1:B:351:PRO:HD2	1:B:354:TRP:HB2	1.96	0.47
2:C:138:VAL:HG21	3:D:136:LEU:HD11	1.95	0.47
2:E:127:ASP:HA	2:E:130:LEU:HD12	1.95	0.47
3:F:171:LEU:HD12	3:F:171:LEU:HA	1.75	0.47
3:F:6:GLU:OE2	3:F:118:GLY:N	2.46	0.47
2:C:172:ASP:HB3	2:C:175:ASP:OD2	2.14	0.47
3:F:32:TYR:HA	4:F:305:HOH:O	2.13	0.47
3:F:135:PRO:O	3:F:136:LEU:HD23	2.14	0.47
1:A:356:SER:HB3	1:A:362:ARG:CG	2.36	0.47
3:D:172:THR:O	3:D:175:VAL:HG12	2.15	0.47
2:E:188:LYS:HE3	2:E:192:GLU:CD	2.33	0.47
1:A:334:TRP:CZ3	1:A:335:ILE:HG12	2.50	0.47
3:F:59:TYR:CE1	3:F:69:ILE:HG13	2.49	0.47
1:A:309:CYS:SG	1:A:318:CYS:CB	3.03	0.47
1:B:403:LEU:HB2	1:B:406:MET:HG3	1.97	0.47
1:A:367:TYR:CE2	1:B:324:ILE:HD13	2.46	0.47
2:C:124:PRO:HB3	2:C:214:PHE:CE2	2.50	0.47
3:D:200:SER:HA	3:D:203:THR:HB	1.96	0.47
2:E:136:SER:HA	2:E:184:LEU:O	2.15	0.47
2:E:137:VAL:HG22	2:E:184:LEU:HB3	1.96	0.47
3:F:36:TRP:HD1	3:F:69:ILE:HD13	1.79	0.47
3:F:128:THR:HG21	3:F:214:PRO:O	2.15	0.47
3:D:81:GLN:OE1	3:D:83:ASN:ND2	2.43	0.47
1:B:375:SER:OG	1:B:376:ALA:N	2.44	0.46
2:C:125:PRO:HB2	2:C:130:LEU:HD21	1.96	0.46
2:E:155:VAL:HG12	2:E:197:TYR:CD1	2.49	0.46
3:D:86:ARG:HD3	4:D:302:HOH:O	2.16	0.46
3:D:88:GLU:OE1	3:D:88:GLU:N	2.39	0.46
2:E:171:GLN:HG3	2:E:176:SER:HA	1.96	0.46
1:A:330:LEU:HD23	1:B:366:LEU:HD23	1.98	0.46
2:E:190:ASP:N	2:E:190:ASP:OD2	2.49	0.46
3:D:86:ARG:CD	4:D:302:HOH:O	2.64	0.46
3:D:221:LYS:HD2	3:D:221:LYS:HA	1.49	0.45
2:C:127:ASP:HA	2:C:130:LEU:HD12	1.99	0.45
3:F:201:LEU:HD13	3:F:206:TYR:CD2	2.50	0.45
2:E:188:LYS:O	2:E:192:GLU:HG2	2.16	0.45
1:B:357:ASP:HB3	1:B:361:SER:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:HIS:HB3	3:D:217:THR:HG1	1.77	0.45
1:A:392:TYR:CD1	1:A:399:LYS:HD3	2.52	0.45
2:E:130:LEU:C	2:E:132:SER:H	2.21	0.45
2:E:154:LYS:CE	2:E:157:ASN:HA	2.47	0.45
2:C:85:PHE:CZ	2:C:170:GLU:HB3	2.52	0.44
3:D:6:GLU:OE1	3:D:95:CYS:N	2.50	0.44
1:B:386:GLU:HG2	1:B:387:PRO:HD2	2.00	0.44
3:D:11:LEU:HD11	3:D:124:SER:OG	2.17	0.44
3:F:128:THR:HG23	3:F:159:PRO:HD3	1.98	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.78	0.44
3:D:27:PHE:HB2	3:D:32:TYR:CD2	2.53	0.44
2:E:202:THR:HG22	2:E:209:PRO:HG3	1.99	0.44
3:F:3:GLN:C	3:F:4:LEU:HD12	2.37	0.44
3:D:151:GLY:HA2	3:D:166:TRP:CH2	2.52	0.44
2:E:113:ARG:HG3	2:E:176:SER:OG	2.18	0.44
1:A:392:TYR:CE1	1:A:399:LYS:HD3	2.53	0.44
1:B:309:CYS:HG	1:B:318:CYS:CB	2.24	0.44
3:D:87:ALA:HA	3:D:123:VAL:HG23	1.99	0.44
3:D:222:LYS:HB2	3:D:222:LYS:HE2	1.76	0.44
3:D:154:VAL:CG2	3:D:210:VAL:HG21	2.46	0.44
3:D:207:ILE:CB	3:D:221:LYS:O	2.57	0.44
1:A:393:TYR:O	1:A:395:GLY:N	2.51	0.43
3:D:15:GLY:HA2	3:D:84:SER:HA	2.00	0.43
1:B:325:ASP:O	1:B:329:ASP:HB2	2.17	0.43
3:D:200:SER:O	3:D:202:GLY:N	2.51	0.43
2:C:82:PRO:HA	2:C:111:ILE:HG13	2.01	0.43
1:B:399:LYS:HD3	1:B:400:ILE:H	1.84	0.43
3:F:11:LEU:HD12	3:F:12:VAL:H	1.83	0.43
2:E:128:GLU:OE1	3:F:221:LYS:NZ	2.52	0.43
1:B:364:LEU:HD23	1:B:364:LEU:HA	1.84	0.43
2:C:83:GLU:CD	2:C:83:GLU:H	2.22	0.43
2:C:123:PHE:HA	2:C:124:PRO:HD3	1.84	0.43
3:F:50:TYR:CD1	3:F:50:TYR:C	2.91	0.43
3:F:221:LYS:HD3	3:F:222:LYS:O	2.18	0.43
3:D:27:PHE:HB2	3:D:32:TYR:CE2	2.54	0.43
3:F:20:LEU:HD12	3:F:20:LEU:N	2.33	0.43
1:A:341:TYR:HE2	1:A:407:ILE:HG13	1.83	0.42
2:C:69:SER:OG	2:C:70:GLY:N	2.51	0.42
2:C:124:PRO:HB3	2:C:214:PHE:CZ	2.54	0.42
2:E:145:TYR:CD1	2:E:146:PRO:HA	2.54	0.42
3:F:40:ALA:HB3	3:F:43:LYS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASP:HB3	1:B:361:SER:HB2	2.01	0.42
1:B:385:LEU:HD13	1:B:405:ASN:HB3	2.01	0.42
2:E:34:TYR:CD1	3:F:109:MET:HA	2.54	0.42
2:E:188:LYS:CD	2:E:192:GLU:OE1	2.67	0.42
1:B:324:ILE:HG21	1:B:330:LEU:HD11	2.01	0.42
1:A:401:GLU:CG	1:A:402:GLN:N	2.83	0.42
3:D:50:TYR:CD1	3:D:50:TYR:C	2.93	0.42
2:E:148:GLU:OE2	2:E:148:GLU:N	2.41	0.42
2:E:188:LYS:HE3	2:E:192:GLU:OE1	2.19	0.42
3:F:150:LEU:HD12	3:F:151:GLY:N	2.34	0.42
1:B:314:GLN:HG3	1:B:315:ASP:N	2.35	0.42
3:D:32:TYR:CZ	3:D:101:VAL:HG12	2.55	0.42
3:F:150:LEU:HD11	3:F:166:TRP:CZ3	2.55	0.42
3:F:133:VAL:CG2	3:F:210:VAL:HG11	2.37	0.42
2:E:126:SER:O	2:E:130:LEU:HG	2.20	0.41
1:A:323:TYR:CZ	1:A:340:GLY:HA3	2.55	0.41
3:D:11:LEU:HD12	3:D:11:LEU:HA	1.83	0.41
3:D:174:GLY:O	3:D:194:VAL:HA	2.21	0.41
3:F:6:GLU:OE2	3:F:94:PHE:HA	2.20	0.41
3:F:48:ILE:HG21	3:F:48:ILE:HD13	1.79	0.41
3:F:67:PHE:CE2	3:F:82:MET:HB3	2.54	0.41
1:B:341:TYR:CZ	1:B:343:ALA:HB2	2.56	0.41
3:D:59:TYR:OH	3:D:68:THR:HA	2.21	0.41
3:F:19:ARG:HB2	3:F:81:GLN:HE22	1.83	0.41
3:D:90:THR:HG22	3:D:123:VAL:H	1.84	0.41
2:E:123:PHE:HB3	3:F:136:LEU:HB3	2.01	0.41
1:B:384:ASP:HB2	1:B:410:SER:OG	2.21	0.41
3:D:136:LEU:HD23	3:D:136:LEU:HA	1.75	0.41
2:E:145:TYR:CG	2:E:146:PRO:HA	2.54	0.41
3:F:50:TYR:HE1	3:F:52:SER:HB3	1.86	0.41
1:B:357:ASP:CG	1:B:358:THR:H	2.23	0.41
2:C:126:SER:CB	3:D:135:PRO:HG2	2.50	0.41
2:E:25:SER:O	2:E:71:THR:OG1	2.39	0.41
2:E:154:LYS:HE2	2:E:158:ALA:N	2.35	0.41
2:E:201:VAL:HG13	2:E:206:LEU:HD21	2.03	0.41
3:F:67:PHE:HD2	3:F:80:LEU:HD11	1.85	0.41
3:F:160:GLU:OE1	3:F:161:PRO:HA	2.21	0.41
3:D:4:LEU:HD22	3:D:95:CYS:SG	2.60	0.41
2:E:203:HIS:HB3	2:E:206:LEU:CD1	2.50	0.41
1:A:401:GLU:HG2	1:A:402:GLN:N	2.36	0.41
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:47:TRP:HZ2	3:F:50:TYR:CD2	2.38	0.41
3:F:207:ILE:HD12	3:F:221:LYS:O	2.20	0.41
1:B:409:LYS:HA	1:B:409:LYS:HD2	1.97	0.40
3:D:20:LEU:HD12	3:D:80:LEU:HD23	2.02	0.40
1:A:322:LEU:HD11	1:B:367:TYR:CE1	2.57	0.40
3:D:51:ILE:HB	3:D:69:ILE:HG22	2.03	0.40
2:E:180:LEU:HD12	2:E:181:SER:N	2.34	0.40
3:F:35:ASN:OD1	3:F:98:HIS:HE1	2.04	0.40
2:E:25:SER:OG	2:E:27:GLN:O	2.24	0.40
2:C:33:ASN:HD21	3:D:109:MET:CE	2.34	0.40
2:E:80:LEU:HD23	2:E:80:LEU:HA	1.77	0.40
2:E:126:SER:C	2:E:128:GLU:H	2.23	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	107/112 (96%)	93 (87%)	11 (10%)	3 (3%)	5	19
1	B	110/112 (98%)	103 (94%)	6 (6%)	1 (1%)	17	48
2	C	215/219 (98%)	198 (92%)	13 (6%)	4 (2%)	8	28
2	E	198/219 (90%)	174 (88%)	22 (11%)	2 (1%)	15	45
3	D	212/233 (91%)	203 (96%)	8 (4%)	1 (0%)	29	61
3	F	212/233 (91%)	187 (88%)	22 (10%)	3 (1%)	11	36
All	All	1054/1128 (93%)	958 (91%)	82 (8%)	14 (1%)	12	37

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	169	THR

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Mol	Chain	Res	Type
1	A	394	ILE
2	E	70	GLY
2	C	132	SER
3	D	201	LEU
1	A	358	THR
2	C	95	SER
3	F	125	SER
2	C	70	GLY
3	F	167	ASN
1	B	351	PRO
2	C	217	GLY
3	F	213	LYS
1	A	400	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/100 (99%)	94 (95%)	5 (5%)	24	56
1	B	100/100 (100%)	98 (98%)	2 (2%)	55	82
2	C	187/189 (99%)	176 (94%)	11 (6%)	19	49
2	E	177/189 (94%)	167 (94%)	10 (6%)	21	52
3	D	175/190 (92%)	161 (92%)	14 (8%)	12	33
3	F	175/190 (92%)	167 (95%)	8 (5%)	27	60
All	All	913/958 (95%)	863 (94%)	50 (6%)	21	53

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	SER
1	A	366	LEU
1	A	392	TYR
1	A	403	LEU
1	A	404	SER

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Mol	Chain	Res	Type
1	B	308	TYR
1	B	399	LYS
2	C	18	ARG
2	C	23	CYS
2	C	41	LYS
2	C	79	SER
2	C	90	CYS
2	C	121	PHE
2	C	132	SER
2	C	147	ARG
2	C	190	ASP
2	C	204	GLN
2	C	207	SER
3	D	6	GLU
3	D	28	SER
3	D	50	TYR
3	D	56	SER
3	D	81	GLN
3	D	84	SER
3	D	155	LYS
3	D	192	SER
3	D	199	SER
3	D	200	SER
3	D	209	ASN
3	D	213	LYS
3	D	221	LYS
3	D	222	LYS
2	E	85	PHE
2	E	113	ARG
2	E	152	GLN
2	E	154	LYS
2	E	161	SER
2	E	165	GLN
2	E	166	GLU
2	E	182	SER
2	E	190	ASP
2	E	206	LEU
3	F	19	ARG
3	F	82	MET
3	F	83	ASN
3	F	98	HIS
3	F	192	SER

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Mol	Chain	Res	Type
3	F	209	ASN
3	F	220	ASP
3	F	221	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	314	GLN
1	B	360	HIS
2	C	33	ASN
2	E	142	ASN
2	E	143	ASN
2	E	163	ASN
3	F	81	GLN
3	F	209	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 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	111/112 (99%)	0.01	3 (2%) 54 50	54, 78, 120, 131	0
1	B	112/112 (100%)	-0.24	0 100 100	50, 66, 82, 94	0
2	C	217/219 (99%)	-0.35	0 100 100	52, 69, 99, 110	0
2	E	204/219 (93%)	0.08	11 (5%) 25 22	36, 78, 121, 127	0
3	D	216/233 (92%)	-0.16	3 (1%) 75 75	48, 71, 112, 123	0
3	F	216/233 (92%)	-0.14	2 (0%) 84 84	49, 81, 116, 133	0
All	All	1076/1128 (95%)	-0.14	19 (1%) 68 67	36, 72, 114, 133	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	170	ALA	4.7
2	E	122	ILE	3.7
2	E	193	LYS	3.4
2	E	153	TRP	3.3
2	E	151	VAL	3.2
2	E	124	PRO	2.9
2	E	117	ALA	2.9
1	A	394	ILE	2.7
1	A	393	TYR	2.6
3	D	171	LEU	2.6
1	A	354	TRP	2.4
3	F	222	LYS	2.3
3	F	223	VAL	2.3
2	E	164	SER	2.3
2	E	141	LEU	2.2
2	E	188	LYS	2.2
2	E	201	VAL	2.2
3	D	148	ALA	2.1
2	E	187	SER	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.