Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 02:40 AM EDT

PDB ID	:	5YWF
Title	:	Crystal structure of 2H4 Fab
Authors	:	Qiu, X.; Lei, Y.; Yang, P.; Gao, Q.; Wang, N.; Cao, L.; Wang, X.; Xu, Z.K.; Rao, Z.
Deposited on	:	2017-11-29
Resolution	:	2.21 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 (i) 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 (1)) were used in the production of this report:

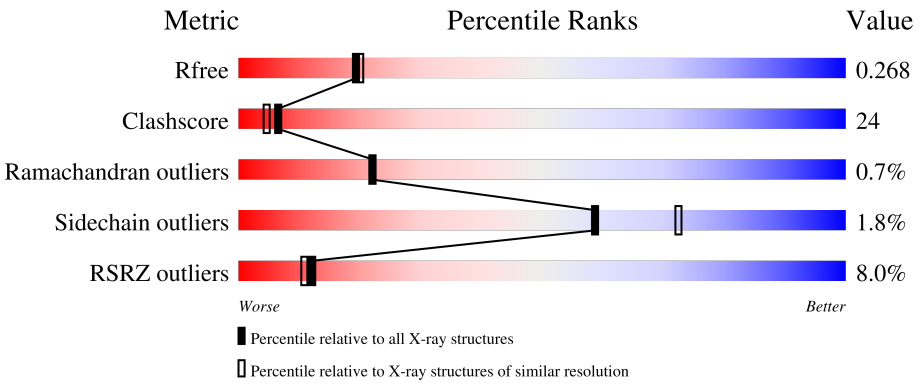
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.21 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	215	6% 60% 33% 6% •
1	C	215	10% 68% 30% •
2	B	218	2% 72% 27% •
2	D	218	14% 76% 22% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6772 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 2H4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1657	1029	287	334	7	0	0	0
1	C	215	1647	1022	283	336	6	0	0	0

- Molecule 2 is a protein called 2H4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1633	1041	264	320	8	0	0	0
2	D	218	1628	1037	262	320	9	0	0	0

- Molecule 3 is water.

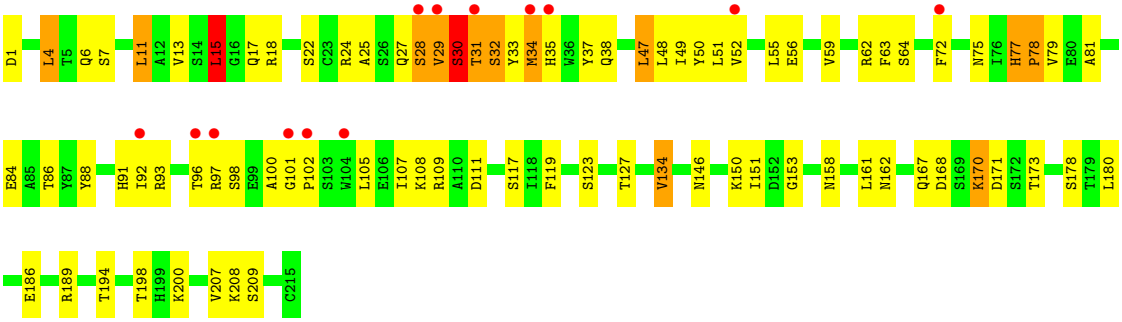
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0
3	B	61	61	61	0	0
3	C	46	46	46	0	0
3	D	42	42	42	0	0

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.

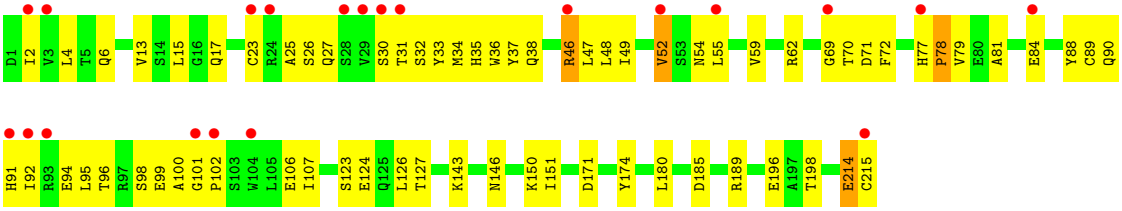
- Molecule 1: 2H4 light chain

Chain A:



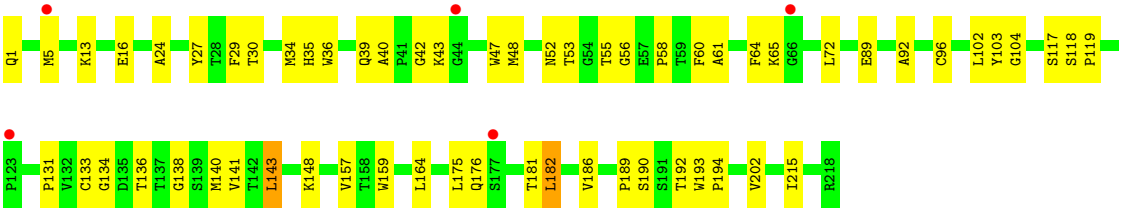
- Molecule 1: 2H4 light chain

Chain C:



- Molecule 2: 2H4 heavy chain

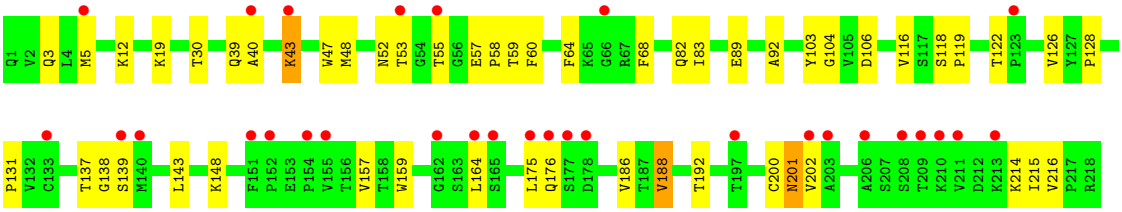
Chain B:



- Molecule 2: 2H4 heavy chain

Chain D:

14%
76%
22%


Q1 V2 Q3 L4 M5 K12 K19 T30 Q39 A40 K43 W47 M48 N52 T53 G54 T55 G56 E57 P58 T59 F60 F64 K65 G66 R67 F68 Q82 I83 E89 A92 Y103 G104 V105 D106 V116 S117 S118 P119 T122 P123 V126 Y127 P128
P131 V132 C133 T137 G138 S139 M140 L143 K148 F151 P152 E153 P154 V155 T156 V157 T158 W159 G162 S163 L164 S165 L175 Q176 S177 D178 V186 T187 V188 T192 T197 C200 N201 V202 A203 A206 S207 S208 T209 K210 V211 D212 K213 K214 I215 V216 P217 R218

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.37Å 140.98Å 78.96Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	44.36 – 2.21 44.36 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.36-2.21) 99.4 (44.36-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.215 , 0.262 0.230 , 0.268	Depositor DCC
R_{free} test set	2379 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6772	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 (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	0.58	0/1696	0.82	7/2309 (0.3%)
1	C	0.63	4/1686 (0.2%)	0.72	2/2297 (0.1%)
2	B	0.46	0/1680	0.70	1/2299 (0.0%)
2	D	0.46	1/1675 (0.1%)	0.66	0/2294
All	All	0.54	5/6737 (0.1%)	0.73	10/9199 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	ARG	NE-CZ	-10.43	1.19	1.33
1	C	46	ARG	CZ-NH2	-9.29	1.21	1.33
1	C	46	ARG	CZ-NH1	-9.07	1.21	1.33
1	C	46	ARG	CD-NE	-7.70	1.33	1.46
2	D	188	VAL	CB-CG1	-5.90	1.40	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	VAL	N-CA-C	-9.46	85.47	111.00
1	C	15	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	A	32	SER	N-CA-C	-6.43	93.64	111.00
1	A	15	LEU	CB-CG-CD2	-6.10	100.63	111.00
2	B	182	LEU	CB-CG-CD2	-6.01	100.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	LEU	CB-CG-CD1	5.39	120.17	111.00
1	A	34	MET	CB-CG-SD	-5.33	96.39	112.40
1	A	4	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	C	214	GLU	C-N-CA	5.21	134.73	121.70
1	A	11	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	42	GLY	Peptide
2	D	43	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1657	0	1573	129	0
1	C	1647	0	1549	87	1
2	B	1633	0	1585	80	0
2	D	1628	0	1570	52	1
3	A	58	0	0	2	0
3	B	61	0	0	4	0
3	C	46	0	0	6	0
3	D	42	0	0	2	0
All	All	6772	0	6277	304	1

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 24.

All (304) 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:34:MET:SD	1:A:72:PHE:CD1	2.05	1.50
1:C:69:GLY:O	1:C:72:PHE:CZ	1.67	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLY:O	1:C:72:PHE:CE1	1.95	1.18
1:A:31:THR:CG2	1:A:93:ARG:HH21	1.55	1.18
1:A:34:MET:SD	1:A:72:PHE:CE1	2.39	1.15
1:A:47:LEU:HD12	1:A:56:GLU:HG3	1.28	1.15
1:C:92:ILE:HD11	3:C:310:HOH:O	1.47	1.14
2:B:30:THR:HA	2:B:53:THR:CG2	1.77	1.13
1:C:4:LEU:HD11	1:C:91:HIS:CD2	1.90	1.06
1:C:4:LEU:HD11	1:C:91:HIS:HD2	1.20	1.06
1:A:92:ILE:HG21	2:B:104:GLY:N	1.72	1.04
2:B:30:THR:HA	2:B:53:THR:HG21	1.39	1.02
1:C:31:THR:H	1:C:69:GLY:HA2	1.26	1.00
2:D:30:THR:HA	2:D:53:THR:OG1	1.62	0.99
1:C:31:THR:N	1:C:69:GLY:HA2	1.77	0.98
1:A:31:THR:CG2	1:A:93:ARG:NH2	2.25	0.98
2:D:122:THR:OG1	3:D:301:HOH:O	1.80	0.98
1:A:4:LEU:HD11	1:A:91:HIS:HD2	1.28	0.97
1:A:35:HIS:ND1	3:A:301:HOH:O	1.96	0.97
1:A:34:MET:CE	1:A:72:PHE:CE1	2.48	0.96
1:C:69:GLY:O	1:C:72:PHE:HZ	1.32	0.95
2:B:148:LYS:HA	2:B:181:THR:HG22	1.47	0.94
2:D:148:LYS:NZ	2:D:176:GLN:HE22	1.63	0.94
1:C:92:ILE:CD1	3:C:310:HOH:O	2.06	0.93
1:A:15:LEU:CD2	2:D:139:SER:HB3	1.99	0.93
1:C:96:THR:HG1	2:D:47:TRP:HE3	0.91	0.90
2:B:30:THR:HA	2:B:53:THR:HG22	1.55	0.89
1:C:92:ILE:HG21	2:D:104:GLY:N	1.88	0.89
1:A:31:THR:HG21	1:A:93:ARG:HH21	1.33	0.89
1:A:4:LEU:HD11	1:A:91:HIS:CD2	2.07	0.89
1:C:96:THR:OG1	2:D:47:TRP:HE3	1.53	0.89
2:B:133:CYS:O	3:B:301:HOH:O	1.92	0.87
1:C:91:HIS:CD2	1:C:98:SER:OG	2.28	0.86
1:A:92:ILE:HG21	2:B:104:GLY:H	1.36	0.86
1:C:96:THR:OG1	2:D:47:TRP:CE3	2.29	0.85
1:C:77:HIS:ND1	1:C:78:PRO:HD3	1.91	0.85
1:A:37:TYR:CE2	1:A:47:LEU:HD23	2.11	0.84
1:A:77:HIS:CG	1:A:78:PRO:HD3	2.14	0.83
1:A:97:ARG:HG2	1:A:97:ARG:HH21	1.40	0.83
1:A:111:ASP:OD2	1:A:200:LYS:NZ	2.11	0.82
1:C:55:LEU:HD12	1:C:55:LEU:O	1.80	0.81
1:A:97:ARG:HE	2:B:35:HIS:CE1	1.98	0.81
1:A:34:MET:SD	1:A:72:PHE:HD1	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:CYS:HG	1:C:89:CYS:HG	0.97	0.80
1:C:77:HIS:CG	1:C:78:PRO:HD3	2.16	0.80
1:A:91:HIS:CD2	1:A:98:SER:OG	2.36	0.79
1:A:107:ILE:H	1:A:167:GLN:HE22	1.31	0.78
2:D:148:LYS:HZ1	2:D:176:GLN:HE22	1.27	0.78
1:A:47:LEU:HD12	1:A:56:GLU:CG	2.12	0.78
1:A:34:MET:HE3	1:A:72:PHE:CE1	2.20	0.77
2:B:34:MET:HE1	2:B:96:CYS:HB2	1.66	0.76
1:A:15:LEU:HD21	2:D:139:SER:CB	2.16	0.75
1:C:88:TYR:CE1	1:C:102:PRO:HB3	2.21	0.74
1:C:35:HIS:CE1	1:C:47:LEU:HD21	2.22	0.74
1:C:35:HIS:NE2	2:D:103:TYR:O	2.21	0.74
1:A:96:THR:HG22	2:B:47:TRP:HZ3	1.54	0.73
1:A:108:LYS:O	2:D:138:GLY:HA3	1.89	0.73
1:C:4:LEU:CD1	1:C:91:HIS:HD2	2.00	0.72
1:A:35:HIS:CE1	2:B:103:TYR:O	2.43	0.72
1:A:208:LYS:HE3	2:B:134:GLY:O	1.90	0.72
1:A:15:LEU:CD2	2:D:139:SER:CB	2.67	0.71
2:B:148:LYS:HG3	2:B:181:THR:CG2	2.20	0.71
1:A:15:LEU:HD23	2:D:139:SER:HB3	1.72	0.71
2:B:176:GLN:NE2	2:B:181:THR:OG1	2.23	0.70
1:A:77:HIS:ND1	1:A:78:PRO:HD3	2.06	0.70
1:A:171:ASP:OD2	1:A:173:THR:OG1	2.10	0.69
1:A:96:THR:HB	2:B:47:TRP:CE3	2.28	0.69
1:C:150:LYS:NZ	1:C:196:GLU:OE1	2.23	0.68
1:C:91:HIS:CD2	1:C:98:SER:HG	2.09	0.68
1:A:34:MET:CE	1:A:72:PHE:HE1	2.06	0.68
1:A:92:ILE:CD1	2:B:104:GLY:HA3	2.24	0.68
2:B:52:ASN:HD22	2:B:55:THR:HB	1.59	0.68
2:D:40:ALA:HB3	2:D:43:LYS:H	1.58	0.68
1:A:29:VAL:C	1:A:31:THR:H	1.96	0.67
1:C:185:ASP:O	1:C:189:ARG:HG3	1.95	0.67
1:A:194:THR:OG1	1:A:209:SER:HB2	1.95	0.67
1:A:123:SER:O	1:A:127:THR:HG23	1.95	0.67
2:B:29:PHE:O	2:B:53:THR:HG21	1.94	0.67
2:B:141:VAL:HG13	2:B:190:SER:HB3	1.75	0.67
2:D:175:LEU:C	2:D:175:LEU:HD23	2.14	0.67
1:A:86:THR:HG22	1:A:102:PRO:HB2	1.76	0.66
1:A:31:THR:HG23	1:A:93:ARG:NH2	2.11	0.66
1:C:81:ALA:O	1:C:84:GLU:HG2	1.95	0.66
2:B:30:THR:CA	2:B:53:THR:HG21	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG22	1:A:93:ARG:NH2	2.10	0.66
1:A:37:TYR:CD2	1:A:47:LEU:HD23	2.32	0.65
1:A:49:ILE:CD1	1:A:55:LEU:HD23	2.27	0.65
2:B:131:PRO:HD3	2:B:143:LEU:HD12	1.79	0.64
1:A:91:HIS:NE2	1:A:98:SER:OG	2.30	0.64
2:B:157:VAL:HG22	2:B:202:VAL:HG22	1.79	0.64
1:A:15:LEU:HA	1:A:79:VAL:HG23	1.78	0.63
1:C:2:ILE:HG21	1:C:94:GLU:OE2	1.98	0.63
2:B:175:LEU:O	2:B:176:GLN:HG3	1.98	0.63
2:D:148:LYS:HZ2	2:D:176:GLN:HE22	1.45	0.63
1:A:55:LEU:HD21	1:A:63:PHE:O	1.99	0.62
1:A:34:MET:SD	1:A:72:PHE:CG	2.85	0.62
1:A:97:ARG:HH21	1:A:97:ARG:CG	2.11	0.62
1:A:93:ARG:O	1:A:93:ARG:HD3	1.99	0.62
1:A:92:ILE:HB	2:B:102:LEU:O	2.00	0.62
2:D:39:GLN:O	2:D:92:ALA:HB1	1.99	0.62
2:B:30:THR:OG1	3:B:302:HOH:O	2.16	0.62
2:B:159:TRP:HZ3	2:B:215:ILE:HD11	1.64	0.62
1:A:92:ILE:HD12	2:B:104:GLY:CA	2.30	0.62
1:A:168:ASP:OD1	1:A:170:LYS:HD2	2.01	0.61
1:A:92:ILE:HD12	2:B:104:GLY:HA3	1.83	0.61
1:C:70:THR:HG23	1:C:71:ASP:OD1	2.00	0.61
1:A:27:GLN:HG3	1:A:28:SER:N	2.15	0.61
1:C:2:ILE:CG2	1:C:94:GLU:OE2	2.48	0.61
1:C:123:SER:O	1:C:127:THR:HG23	2.01	0.60
1:C:38:GLN:NE2	1:C:46:ARG:HH21	1.99	0.60
2:D:3:GLN:HB3	2:D:5:MET:SD	2.42	0.60
1:A:31:THR:OG1	1:A:32:SER:N	2.33	0.59
2:B:141:VAL:CG1	2:B:190:SER:HB3	2.32	0.59
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.84	0.59
1:A:81:ALA:O	1:A:84:GLU:HG2	2.02	0.59
1:C:37:TYR:CE2	1:C:47:LEU:HD13	2.37	0.59
1:A:48:LEU:HA	1:A:59:VAL:HG11	1.83	0.59
1:A:92:ILE:HG13	2:B:103:TYR:C	2.23	0.59
1:A:119:PHE:HB2	1:A:134:VAL:HG22	1.84	0.58
1:C:91:HIS:NE2	1:C:98:SER:OG	2.23	0.58
2:B:13:LYS:N	2:B:16:GLU:OE1	2.25	0.58
1:C:2:ILE:HG13	1:C:26:SER:OG	2.04	0.57
1:C:38:GLN:HE22	1:C:46:ARG:HH21	1.52	0.57
1:A:29:VAL:HG12	1:A:29:VAL:O	2.03	0.57
2:B:56:GLY:HA2	2:B:72:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASN:HB3	1:C:198:THR:CG2	2.34	0.57
2:B:175:LEU:C	2:B:176:GLN:HG3	2.25	0.57
2:D:19:LYS:HD3	2:D:82:GLN:HB2	1.87	0.57
2:B:148:LYS:HG3	2:B:181:THR:HG21	1.86	0.56
1:C:37:TYR:CD2	1:C:47:LEU:HD13	2.41	0.56
2:D:131:PRO:HD3	2:D:143:LEU:HD22	1.87	0.56
1:A:108:LYS:O	2:D:138:GLY:CA	2.52	0.56
2:B:55:THR:O	2:B:55:THR:HG22	2.04	0.56
1:C:32:SER:O	1:C:33:TYR:C	2.44	0.56
1:C:32:SER:O	1:C:34:MET:N	2.39	0.56
2:B:176:GLN:OE1	2:B:181:THR:HG23	2.05	0.56
1:C:106:GLU:HG2	1:C:107:ILE:N	2.21	0.56
1:A:13:VAL:HG23	1:A:17:GLN:NE2	2.21	0.55
1:C:2:ILE:HA	1:C:26:SER:OG	2.06	0.55
1:A:4:LEU:CD1	1:A:91:HIS:HD2	2.11	0.55
1:A:47:LEU:HD13	1:A:48:LEU:N	2.21	0.55
1:A:34:MET:C	1:A:35:HIS:CD2	2.80	0.55
1:C:31:THR:H	1:C:69:GLY:CA	2.11	0.55
2:B:36:TRP:HB3	2:B:48:MET:CE	2.37	0.54
1:A:194:THR:OG1	1:A:209:SER:CB	2.54	0.54
1:C:13:VAL:CG2	1:C:79:VAL:HG11	2.38	0.54
1:C:47:LEU:HD22	2:D:106:ASP:HA	1.88	0.54
1:A:27:GLN:CG	1:A:28:SER:N	2.71	0.54
1:C:69:GLY:C	1:C:72:PHE:CZ	2.71	0.54
1:C:77:HIS:CE1	1:C:78:PRO:HD3	2.42	0.53
1:C:146:ASN:HB3	1:C:198:THR:HG22	1.89	0.53
2:D:126:VAL:HG21	2:D:202:VAL:HG21	1.89	0.53
1:A:146:ASN:HB3	1:A:198:THR:HG22	1.90	0.53
1:A:146:ASN:HB3	1:A:198:THR:CG2	2.39	0.53
2:B:159:TRP:HZ3	2:B:215:ILE:CD1	2.21	0.53
2:B:148:LYS:HG3	2:B:181:THR:HG22	1.90	0.52
2:B:89:GLU:N	2:B:89:GLU:OE2	2.43	0.52
2:B:159:TRP:CZ3	2:B:215:ILE:HD11	2.43	0.52
1:A:97:ARG:CG	1:A:97:ARG:NH2	2.72	0.52
1:A:55:LEU:HB3	1:A:59:VAL:HG22	1.92	0.51
2:B:138:GLY:HA2	1:C:107:ILE:HG12	1.92	0.51
1:C:124:GLU:OE2	1:C:124:GLU:N	2.44	0.51
2:D:157:VAL:HG22	2:D:202:VAL:HG12	1.92	0.51
1:A:161:LEU:CD1	2:B:176:GLN:HG2	2.41	0.51
1:A:92:ILE:HG21	2:B:104:GLY:CA	2.40	0.50
1:A:96:THR:HB	2:B:47:TRP:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:OE1	1:A:107:ILE:HB	2.12	0.50
1:C:36:TRP:O	1:C:47:LEU:HD12	2.11	0.50
1:A:92:ILE:CG2	2:B:104:GLY:N	2.59	0.50
2:B:61:ALA:O	2:B:65:LYS:HG3	2.12	0.50
2:B:136:THR:HG23	2:B:141:VAL:HG12	1.93	0.50
1:C:30:SER:HB3	1:C:69:GLY:C	2.32	0.50
1:A:151:ILE:HD11	1:A:180:LEU:HD21	1.94	0.50
1:A:97:ARG:HE	2:B:35:HIS:HE1	1.53	0.50
1:A:171:ASP:OD1	1:A:171:ASP:N	2.37	0.50
1:A:49:ILE:HD11	1:A:55:LEU:HD23	1.94	0.50
2:D:148:LYS:HZ1	2:D:176:GLN:NE2	2.02	0.50
2:D:12:LYS:O	2:D:116:VAL:HA	2.13	0.49
1:A:86:THR:CG2	1:A:102:PRO:HB2	2.41	0.49
2:B:48:MET:HA	2:B:64:PHE:CD2	2.47	0.49
2:D:30:THR:HA	2:D:53:THR:HG1	1.76	0.49
1:C:38:GLN:NE2	1:C:46:ARG:NH2	2.59	0.49
2:D:68:PHE:CD2	2:D:83:ILE:HG12	2.48	0.49
2:B:48:MET:HG2	2:B:64:PHE:CZ	2.48	0.49
1:C:90:GLN:CB	3:C:341:HOH:O	2.60	0.49
2:D:118:SER:N	2:D:119:PRO:HD3	2.27	0.49
1:C:38:GLN:HE22	1:C:46:ARG:NH2	2.11	0.48
1:A:7:SER:HB3	1:A:24:ARG:HH22	1.78	0.48
2:D:148:LYS:NZ	2:D:176:GLN:NE2	2.47	0.48
1:A:6:GLN:HB2	1:A:101:GLY:O	2.14	0.48
2:B:193:TRP:CG	2:B:194:PRO:HA	2.48	0.48
2:B:34:MET:CE	2:B:96:CYS:HB2	2.38	0.48
2:D:164:LEU:HD13	2:D:186:VAL:HG21	1.96	0.47
1:C:151:ILE:HD11	1:C:180:LEU:HD21	1.96	0.47
2:B:52:ASN:HD22	2:B:55:THR:CB	2.26	0.47
1:C:36:TRP:CZ3	1:C:89:CYS:HB3	2.49	0.47
1:C:55:LEU:HD12	1:C:55:LEU:C	2.33	0.47
2:D:128:PRO:HB3	2:D:215:ILE:HD13	1.97	0.47
1:A:35:HIS:CE1	1:A:50:TYR:HA	2.50	0.47
1:C:46:ARG:NH1	3:C:308:HOH:O	2.47	0.47
1:A:150:LYS:NZ	1:A:153:GLY:O	2.44	0.47
1:A:88:TYR:CE2	1:A:102:PRO:HB3	2.50	0.47
1:C:92:ILE:HG21	2:D:104:GLY:H	1.74	0.47
2:B:39:GLN:NE2	3:B:306:HOH:O	2.48	0.46
1:C:4:LEU:HD23	1:C:25:ALA:HA	1.97	0.46
1:C:6:GLN:HG3	1:C:100:ALA:HB3	1.96	0.46
2:B:36:TRP:HB3	2:B:48:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:LEU:N	1:C:95:LEU:HD12	2.31	0.46
1:A:77:HIS:CE1	1:A:78:PRO:HD3	2.50	0.46
1:C:62:ARG:HA	1:C:77:HIS:ND1	2.31	0.46
1:A:1:ASP:N	3:A:303:HOH:O	2.28	0.46
1:A:92:ILE:HG22	1:A:92:ILE:O	2.16	0.46
1:C:48:LEU:HA	1:C:59:VAL:HG21	1.98	0.46
2:D:188:VAL:CG1	2:D:192:THR:HB	2.46	0.46
1:A:15:LEU:HD21	2:D:139:SER:HB2	1.95	0.46
1:A:162:ASN:HD22	1:A:178:SER:HA	1.81	0.46
2:D:89:GLU:CD	2:D:89:GLU:H	2.20	0.46
1:C:6:GLN:HG3	1:C:100:ALA:CB	2.46	0.45
1:C:13:VAL:HG21	1:C:79:VAL:HG11	1.96	0.45
1:A:4:LEU:HD23	1:A:25:ALA:HA	1.98	0.45
1:A:35:HIS:ND1	1:A:50:TYR:HA	2.31	0.45
1:C:2:ILE:HG23	1:C:2:ILE:O	2.15	0.45
1:A:55:LEU:HD22	1:A:59:VAL:CG2	2.47	0.45
1:A:92:ILE:CG2	2:B:104:GLY:CA	2.94	0.45
2:B:136:THR:HG23	2:B:140:MET:O	2.16	0.45
2:D:48:MET:HA	2:D:64:PHE:CD2	2.52	0.45
1:A:30:SER:HA	1:A:93:ARG:HG2	1.97	0.45
1:C:88:TYR:CZ	1:C:102:PRO:HB3	2.51	0.45
1:A:27:GLN:CG	1:A:28:SER:H	2.29	0.45
2:D:55:THR:HG22	2:D:57:GLU:HB2	1.98	0.45
2:D:214:LYS:HG2	2:D:216:VAL:HG13	1.99	0.45
1:A:107:ILE:HD11	2:D:139:SER:OG	2.17	0.45
2:B:5:MET:O	2:B:5:MET:HG3	2.16	0.45
1:C:143:LYS:HE2	1:C:143:LYS:HB2	1.68	0.45
1:A:6:GLN:HG3	1:A:100:ALA:CB	2.47	0.45
2:B:58:PRO:HB2	2:B:60:PHE:CE2	2.51	0.45
1:A:17:GLN:O	1:A:79:VAL:HG22	2.17	0.44
1:C:6:GLN:HB2	1:C:101:GLY:O	2.17	0.44
1:C:52:VAL:CB	3:C:318:HOH:O	2.65	0.44
1:A:92:ILE:HD12	2:B:104:GLY:HA2	1.98	0.44
2:B:189:PRO:HG2	2:B:192:THR:HG23	1.99	0.44
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.80	0.44
2:B:118:SER:N	2:B:119:PRO:HD3	2.33	0.44
2:D:59:THR:HG23	3:D:317:HOH:O	2.17	0.44
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.52	0.44
2:D:52:ASN:HB3	2:D:55:THR:HB	1.99	0.44
2:D:55:THR:CG2	2:D:57:GLU:HB2	2.47	0.44
1:A:194:THR:HG23	1:A:208:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:HIS:HE1	1:C:47:LEU:HD21	1.77	0.44
1:A:34:MET:C	1:A:35:HIS:HD2	2.19	0.44
1:C:2:ILE:CG2	1:C:91:HIS:NE2	2.81	0.44
1:A:29:VAL:O	1:A:31:THR:N	2.50	0.44
1:A:35:HIS:HE1	2:B:103:TYR:HB3	1.82	0.44
1:C:90:GLN:CB	1:C:99:GLU:HG3	2.48	0.44
2:D:55:THR:HG22	2:D:57:GLU:CB	2.48	0.44
1:A:194:THR:CG2	1:A:207:VAL:HG13	2.48	0.44
1:A:37:TYR:CE2	1:A:47:LEU:CD2	2.93	0.43
1:A:91:HIS:O	1:A:91:HIS:CG	2.70	0.43
1:C:91:HIS:O	1:C:91:HIS:CG	2.70	0.43
2:D:55:THR:CG2	2:D:57:GLU:CB	2.96	0.43
2:B:40:ALA:HB3	2:B:43:LYS:CB	2.48	0.43
2:D:57:GLU:HA	2:D:58:PRO:HD3	1.88	0.43
2:B:56:GLY:HA2	2:B:72:LEU:CD1	2.48	0.43
1:A:35:HIS:CE1	2:B:103:TYR:HB3	2.53	0.43
1:A:97:ARG:NE	2:B:35:HIS:CE1	2.78	0.43
1:C:23:CYS:CB	1:C:89:CYS:SG	3.06	0.43
1:A:96:THR:CG2	2:B:47:TRP:HZ3	2.27	0.43
2:B:1:GLN:OE1	2:B:1:GLN:N	2.51	0.43
2:B:39:GLN:O	2:B:92:ALA:HB1	2.19	0.43
1:A:92:ILE:HG13	2:B:104:GLY:HA3	2.00	0.43
1:A:35:HIS:CE1	1:A:50:TYR:HB2	2.53	0.42
1:A:47:LEU:CD1	1:A:56:GLU:HG3	2.21	0.42
2:D:157:VAL:HA	2:D:201:ASN:O	2.19	0.42
1:A:29:VAL:C	1:A:31:THR:N	2.69	0.42
1:A:92:ILE:CG1	2:B:104:GLY:HA3	2.49	0.42
1:C:2:ILE:HD12	1:C:27:GLN:CB	2.50	0.42
1:C:17:GLN:O	1:C:79:VAL:HG12	2.20	0.42
1:A:32:SER:HB3	1:A:51:LEU:O	2.19	0.42
1:A:62:ARG:HA	1:A:77:HIS:ND1	2.33	0.42
2:B:117:SER:HB2	2:B:119:PRO:HD3	2.01	0.42
2:D:48:MET:HG2	2:D:64:PHE:CZ	2.55	0.42
1:C:49:ILE:HA	1:C:54:ASN:O	2.19	0.42
1:A:96:THR:HB	2:B:47:TRP:CZ3	2.54	0.42
1:A:31:THR:OG1	1:A:33:TYR:CD2	2.71	0.42
1:C:47:LEU:HD12	1:C:48:LEU:H	1.85	0.42
1:A:13:VAL:HG22	1:A:79:VAL:HG21	2.02	0.41
1:A:92:ILE:HG13	2:B:104:GLY:N	2.34	0.41
1:C:2:ILE:HG22	1:C:94:GLU:OE2	2.19	0.41
1:C:47:LEU:CD2	2:D:106:ASP:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLN:N	2:B:1:GLN:CD	2.74	0.41
2:D:60:PHE:CE1	2:D:68:PHE:O	2.73	0.41
1:C:69:GLY:O	1:C:72:PHE:HE1	1.85	0.41
1:C:174:TYR:HB3	3:C:315:HOH:O	2.21	0.41
1:A:109:ARG:HD2	1:A:171:ASP:O	2.20	0.41
1:A:186:GLU:O	1:A:189:ARG:HG2	2.21	0.41
2:B:182:LEU:HA	3:B:317:HOH:O	2.20	0.41
2:D:159:TRP:CZ3	2:D:200:CYS:HB3	2.55	0.41
1:A:47:LEU:HD22	1:A:47:LEU:HA	1.80	0.41
1:A:64:SER:HB3	1:A:75:ASN:HB3	2.01	0.41
2:B:164:LEU:HD13	2:B:186:VAL:HG21	2.03	0.41
1:A:11:LEU:HD22	1:A:105:LEU:HD11	2.02	0.40
1:C:92:ILE:O	1:C:92:ILE:HG22	2.21	0.40
1:A:117:SER:HB3	1:A:119:PHE:CE1	2.56	0.40
1:C:171:ASP:OD1	1:C:171:ASP:N	2.46	0.40

All (1) 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)
1:C:214:GLU:OE1	2:D:53:THR:CG2[2_745]	2.18	0.02

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	213/215 (99%)	199 (93%)	10 (5%)	4 (2%)	8 5
1	C	213/215 (99%)	201 (94%)	10 (5%)	2 (1%)	17 16
2	B	216/218 (99%)	205 (95%)	11 (5%)	0	100 100
2	D	216/218 (99%)	206 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	858/866 (99%)	811 (94%)	41 (5%)	6 (1%)	22 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	52	VAL
1	A	78	PRO
1	C	52	VAL
1	C	78	PRO
1	A	30	SER

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	186/192 (97%)	177 (95%)	9 (5%)	25 32
1	C	184/192 (96%)	183 (100%)	1 (0%)	88 94
2	B	183/185 (99%)	182 (100%)	1 (0%)	88 94
2	D	182/185 (98%)	180 (99%)	2 (1%)	73 85
All	All	735/754 (98%)	722 (98%)	13 (2%)	59 72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	ARG
1	A	22	SER
1	A	30	SER
1	A	31	THR
1	A	77	HIS
1	A	134	VAL
1	A	158	ASN
1	A	170	LYS

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Mol	Chain	Res	Type
2	B	143	LEU
1	C	215	CYS
2	D	137	THR
2	D	201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	GLN
1	A	162	ASN
1	A	167	GLN
1	A	213	ASN
2	B	39	GLN
2	B	52	ASN
2	B	176	GLN
1	C	38	GLN
1	C	191	ASN
2	D	176	GLN
2	D	201	ASN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	215/215 (100%)	0.39	13 (6%)	21	20	24, 41, 60, 86	0
1	C	215/215 (100%)	0.67	21 (9%)	7	6	26, 50, 77, 102	0
2	B	218/218 (100%)	0.23	5 (2%)	60	58	23, 39, 63, 74	0
2	D	218/218 (100%)	0.63	30 (13%)	2	2	31, 50, 83, 92	0
All	All	866/866 (100%)	0.48	69 (7%)	12	11	23, 45, 75, 102	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	SER	11.0
1	C	29	VAL	8.7
1	C	31	THR	6.6
1	A	104	TRP	5.8
1	A	29	VAL	5.2
1	C	104	TRP	5.1
2	D	155	VAL	5.0
1	C	84	GLU	4.5
2	D	210	LYS	4.2
2	D	197	THR	4.2
2	D	175	LEU	4.1
1	C	101	GLY	4.1
1	C	69	GLY	3.9
2	D	123	PRO	3.9
2	B	44	GLY	3.9
1	A	34	MET	3.8
1	C	55	LEU	3.6
1	C	30	SER	3.6
2	D	177	SER	3.5
1	A	52	VAL	3.5
2	B	66	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	202	VAL	3.3
2	D	133	CYS	3.3
2	D	209	THR	3.3
1	A	92	ILE	3.2
1	A	97	ARG	3.1
2	D	178	ASP	3.1
1	A	102	PRO	3.1
2	D	5	MET	3.1
1	C	77	HIS	3.0
2	D	206	ALA	3.0
2	B	5	MET	2.9
1	A	31	THR	2.9
1	C	102	PRO	2.8
1	A	72	PHE	2.8
2	D	53	THR	2.8
2	D	140	MET	2.7
2	D	66	GLY	2.7
2	D	162	GLY	2.7
2	D	208	SER	2.6
1	C	92	ILE	2.6
2	D	152	PRO	2.6
1	C	52	VAL	2.6
2	D	40	ALA	2.6
1	C	91	HIS	2.5
1	A	101	GLY	2.5
2	D	151	PHE	2.5
2	D	213	LYS	2.5
1	C	23	CYS	2.5
2	D	154	PRO	2.5
2	D	164	LEU	2.4
2	D	203	ALA	2.4
1	C	2	ILE	2.4
2	D	211	VAL	2.4
2	D	43	LYS	2.4
2	B	123	PRO	2.3
1	A	28	SER	2.3
2	D	55	THR	2.3
2	D	139	SER	2.3
1	A	35	HIS	2.2
1	C	3	VAL	2.2
2	D	176	GLN	2.2
2	B	177	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	215	CYS	2.1
1	C	46	ARG	2.1
1	C	24	ARG	2.1
1	C	93	ARG	2.0
2	D	165	SER	2.0
1	A	96	THR	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 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.