Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID	:	5TSW
Title	:	HIGH RESOLUTION CRYSTAL STRUCTURE OF A HUMAN TNF-ALPHA MUTANT
Authors	:	Cha, S.-S.; Kim, J.-S.; Cho, H.-S.; Oh, B.-H.
Deposited on	:	1999-04-22
Resolution	:	2.50 Å(reported)

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

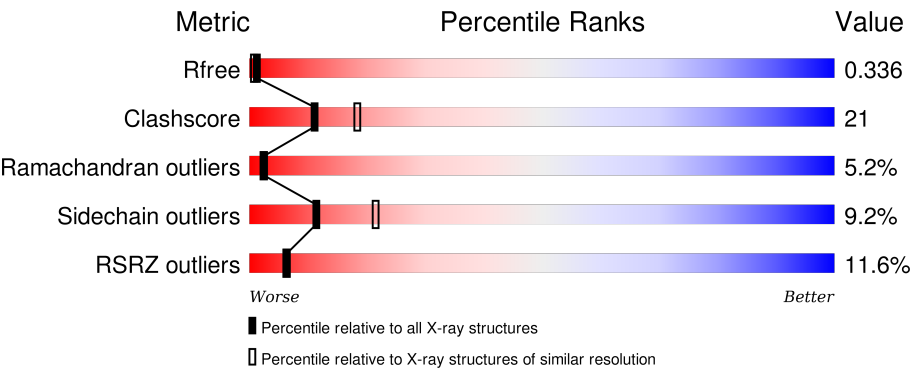|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.336
Clashscore		21
Ramachandran outliers		5.2%
Sidechain outliers		9.2%
RSRZ outliers		11.6%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	150	8% / 53% / 37% / 8% ••
1	B	150	9% / 63% / 30% / 7% •
1	C	150	11% / 53% / 39% / 7% ••
1	D	150	6% / 60% / 31% / 7% ••
1	E	150	16% / 52% / 38% / 8% ••

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Mol	Chain	Length	Quality of chain
1	F	150	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9258 atoms, of which 2182 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 PROTEIN (TUMOR NECROSIS FACTOR-ALPHA).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	149	Total	C	H	N	O	S	0	0	0
			1371	723	245	196	205	2			
1	B	149	Total	C	H	N	O	S	0	0	0
			1363	719	245	196	201	2			
1	C	149	Total	C	H	N	O	S	0	0	0
			1367	721	245	196	203	2			
1	D	149	Total	C	H	N	O	S	0	0	0
			1363	719	245	196	201	2			
1	E	149	Total	C	H	N	O	S	0	0	0
			1363	719	245	196	201	2			
1	F	149	Total	C	H	N	O	S	0	0	0
			1363	719	245	196	201	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	LEU	ENGINEERED	UNP P01375
A	52	ILE	SER	ENGINEERED	UNP P01375
A	56	PHE	TYR	ENGINEERED	UNP P01375
B	29	SER	LEU	ENGINEERED	UNP P01375
B	52	ILE	SER	ENGINEERED	UNP P01375
B	56	PHE	TYR	ENGINEERED	UNP P01375
C	29	SER	LEU	ENGINEERED	UNP P01375
C	52	ILE	SER	ENGINEERED	UNP P01375
C	56	PHE	TYR	ENGINEERED	UNP P01375
D	29	SER	LEU	ENGINEERED	UNP P01375
D	52	ILE	SER	ENGINEERED	UNP P01375
D	56	PHE	TYR	ENGINEERED	UNP P01375
E	29	SER	LEU	ENGINEERED	UNP P01375
E	52	ILE	SER	ENGINEERED	UNP P01375
E	56	PHE	TYR	ENGINEERED	UNP P01375
F	29	SER	LEU	ENGINEERED	UNP P01375
F	52	ILE	SER	ENGINEERED	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
F	56	PHE	TYR	ENGINEERED	UNP P01375

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	57	Total 171	H 114	O 57	0	0
2	B	66	Total 198	H 132	O 66	0	0
2	C	55	Total 165	H 110	O 55	0	0
2	D	62	Total 186	H 124	O 62	0	0
2	E	58	Total 174	H 116	O 58	0	0
2	F	58	Total 174	H 116	O 58	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

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E107 G108 A109 E110 A111 K112 P113 W114 Y115 E116 Y119 L120 F124 E127 D130 R131 L132 S133 I136 P139 L142 D143 F144 I154 I155 A156 L157

• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain E:

16%

52% 38% 8%

PRO S9 D10 K11 P12 Q21 A22 E23 G24 Q25 L26 R31 R32 A33 N34 A35 L36 L37 V41 E42 L43 R44 V49 V50 P51 I52 E53 G54 L55 F56 L57 I58 Y59 S60 Q61 F64 K65 G66 Q67 G68 C69 P70 S71 T72 H73 V74 L75 L76 T77 H78 T79 I80 S81 R82 I83

A84 V85 S86 Y87 Q88 T89 S95 A96 I97 P100 C101 Q102 R103 E104 T105 P106 E107 G108 A109 E110 A111 K112 I118 Y119 L120 G121 L126 E127 K128 G129 D130 R131 L132 S133 I136 P139 D140 Y141 L142 D143 F144 Y151 I155 A156 L157

• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain F:

20%

59% 36%

PRO S9 D10 K11 P12 V13 A14 H15 V16 V17 A18 N19 P20 Q21 A22 L26 Q27 W28 N34 A35 L36 L37 A38 N39 G40 L43 R44 L48 V49 V50 P51 I52 E53 L57 I58 Y59 S60 Q61 V62 Q67 G68 C69 P70 S71 T72 H73 V74 L75 L76 I80 S81 R82 I83

A84 V85 S86 Y87 K90 L94 S95 A96 P100 C101 Q102 R103 E104 T105 P106 E107 G108 A109 E110 A111 K112 Y115 I118 Y119 L120 L126 D130 R131 L132 S133 A134 E135 I136 L142 D143 F144 A145 E146 S147 G148 Q149 V150 I154 I155 A156 L157

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.17Å 94.56Å 95.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.19 – 2.18	Depositor EDS
% Data completeness (in resolution range)	92.5 (8.00-2.50) 85.4 (8.19-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 3.01	Depositor
R, R_{free}	0.207 , 0.299 0.332 , 0.336	Depositor DCC
R_{free} test set	5378 reflections (25.60%)	DCC
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 111.8	EDS
Estimated twinning fraction	0.027 for -h,l,k 0.024 for -l,-k,-h 0.022 for k,h,-l 0.015 for k,l,h 0.015 for l,h,k	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Outliers	0 of 40428 reflections	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	9258	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.65	1/1151 (0.1%)	0.86	2/1569 (0.1%)
1	B	0.61	2/1143 (0.2%)	0.87	2/1559 (0.1%)
1	C	0.60	1/1147 (0.1%)	0.86	2/1564 (0.1%)
1	D	0.65	2/1143 (0.2%)	0.88	2/1559 (0.1%)
1	E	0.73	3/1143 (0.3%)	0.85	0/1559
1	F	0.56	0/1143	0.78	1/1559 (0.1%)
All	All	0.64	9/6870 (0.1%)	0.85	9/9369 (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
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	3
1	F	0	1
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	84	ALA	C-N	-12.30	1.05	1.34
1	A	88	GLN	C-N	-9.97	1.11	1.34
1	D	70	PRO	C-N	-8.99	1.13	1.34
1	E	70	PRO	C-N	-7.87	1.16	1.34
1	B	110	GLU	C-N	-6.80	1.18	1.34
1	C	88	GLN	C-N	-6.42	1.19	1.34
1	E	104	GLU	C-N	6.01	1.47	1.34
1	B	88	GLN	C-N	-5.68	1.21	1.34
1	D	88	GLN	C-N	-5.18	1.22	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	GLU	O-C-N	-10.64	105.67	122.70
1	C	70	PRO	O-C-N	-6.91	111.65	122.70
1	D	84	ALA	O-C-N	-6.68	112.01	122.70
1	D	110	GLU	C-N-CA	5.94	136.55	121.70
1	B	110	GLU	C-N-CA	5.82	136.26	121.70
1	A	84	ALA	O-C-N	-5.58	113.77	122.70
1	C	134	ALA	N-CA-C	-5.33	96.62	111.00
1	A	88	GLN	C-N-CA	5.32	135.00	121.70
1	F	76	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	ALA	Mainchain
1	B	104	GLU	Mainchain
1	B	70	PRO	Mainchain
1	C	70	PRO	Mainchain
1	C	84	ALA	Mainchain
1	D	104	GLU	Mainchain
1	D	119	TYR	Sidechain
1	D	84	ALA	Mainchain
1	F	70	PRO	Mainchain

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	1126	245	1112	43	0
1	B	1118	245	1103	44	1
1	C	1122	245	1108	51	0
1	D	1118	245	1103	57	0
1	E	1118	245	1101	59	1
1	F	1118	245	1105	40	0
2	A	57	114	0	2	5
2	B	66	132	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	55	110	0	1	0
2	D	62	124	0	4	0
2	E	58	116	0	3	0
2	F	58	116	0	4	5
All	All	7076	2182	6632	272	6

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 21.

All (272) 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:B:83:ILE:HD11	1:B:87:TYR:HA	1.21	1.10
1:F:83:ILE:HD12	1:F:87:TYR:HA	1.42	0.99
1:D:58:ILE:HG23	1:D:154:ILE:HG22	1.45	0.97
1:C:76:LEU:HD22	1:C:100:PRO:HD3	1.50	0.93
1:A:53:GLU:HG2	1:A:127:GLU:HA	1.50	0.91
1:A:112:LYS:HD3	1:C:102:GLN:HG3	1.53	0.89
1:F:83:ILE:CD1	1:F:87:TYR:HA	2.04	0.85
1:B:83:ILE:HD11	1:B:87:TYR:CA	2.05	0.85
1:B:76:LEU:HD22	1:B:100:PRO:HD3	1.61	0.83
1:A:69:CYS:O	1:A:104:GLU:HG2	1.79	0.81
1:E:72:THR:HG22	1:E:73:HIS:H	1.43	0.81
1:E:84:ALA:O	1:E:86:SER:N	2.15	0.80
1:E:83:ILE:HB	1:E:131:ARG:HB2	1.66	0.78
1:E:67:GLN:HB2	2:E:1543:HOH:O	1.82	0.77
1:C:14:ALA:HB2	1:C:41:VAL:HG11	1.68	0.76
1:E:111:ALA:HB3	2:E:1543:HOH:O	1.87	0.73
1:B:69:CYS:CB	1:B:101:CYS:HG	2.04	0.71
1:E:12:PRO:HB3	1:E:51:PRO:HG3	1.71	0.71
1:E:50:VAL:HG21	1:E:126:LEU:HD13	1.72	0.71
1:D:76:LEU:HD22	1:D:100:PRO:HD3	1.71	0.71
1:C:74:VAL:HG12	1:C:76:LEU:HD13	1.73	0.70
1:B:90:LYS:HZ2	1:D:70:PRO:HG2	1.57	0.70
1:F:148:GLY:HA2	2:F:263:HOH:O	1.92	0.70
1:C:146:GLU:HB3	1:D:71:SER:HB3	1.74	0.70
1:D:155:ILE:HD13	1:F:157:LEU:HD13	1.74	0.70
1:E:44:ARG:HD3	1:E:49:VAL:HG21	1.75	0.69
1:E:85:VAL:HA	1:E:130:ASP:OD1	1.93	0.69
1:F:58:ILE:HD11	1:F:126:LEU:HD11	1.74	0.69
1:E:26:LEU:HD13	1:E:142:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:LEU:HD22	1:F:100:PRO:HD3	1.75	0.68
1:A:66:GLY:O	1:A:113:PRO:HA	1.93	0.68
1:B:83:ILE:CG2	1:B:131:ARG:HB2	2.24	0.68
1:B:90:LYS:O	1:D:70:PRO:HG3	1.93	0.68
1:A:80:ILE:HA	1:A:133:SER:O	1.96	0.66
1:D:83:ILE:HB	1:D:131:ARG:HB2	1.77	0.66
1:A:69:CYS:O	1:A:71:SER:N	2.27	0.66
1:D:70:PRO:O	1:D:71:SER:HB2	1.96	0.66
1:C:146:GLU:OE2	1:D:72:THR:HA	1.96	0.66
1:C:32:ARG:HD3	1:C:33:ALA:N	2.10	0.66
1:A:76:LEU:HD22	1:A:100:PRO:HD3	1.79	0.65
1:D:112:LYS:HD3	1:F:102:GLN:HG3	1.79	0.65
1:F:69:CYS:HG	1:F:101:CYS:HG	0.67	0.65
1:F:80:ILE:HA	1:F:133:SER:O	1.96	0.64
1:E:70:PRO:O	1:E:71:SER:C	2.34	0.64
1:D:69:CYS:HG	1:D:101:CYS:HG	0.68	0.64
1:B:97:ILE:HD12	1:C:63:LEU:HD21	1.78	0.63
1:E:80:ILE:HA	1:E:133:SER:O	1.98	0.63
1:C:16:VAL:HG12	1:C:30:ASN:HB3	1.80	0.63
1:D:136:ILE:HD11	1:D:139:PRO:HA	1.81	0.63
1:E:11:LYS:HD3	1:E:155:ILE:HD11	1.82	0.62
1:C:82:ARG:HB2	1:C:93:LEU:HD11	1.82	0.62
1:F:81:SER:OG	1:F:90:LYS:HD2	2.00	0.62
1:C:146:GLU:OE2	1:D:72:THR:N	2.33	0.61
1:C:32:ARG:HD3	1:C:33:ALA:H	1.65	0.61
1:D:32:ARG:HD3	2:D:174:HOH:O	1.99	0.61
1:F:69:CYS:CB	1:F:101:CYS:SG	2.89	0.61
1:E:53:GLU:HG2	1:E:54:GLY:N	2.16	0.61
1:F:109:ALA:HB1	1:F:112:LYS:HE2	1.83	0.61
1:B:58:ILE:HD11	1:B:126:LEU:HD11	1.82	0.61
1:D:68:GLY:O	1:D:70:PRO:HD3	2.01	0.61
1:E:60:SER:HB3	1:E:80:ILE:HD11	1.82	0.60
1:E:70:PRO:HG2	1:E:141:TYR:OH	2.02	0.60
1:E:60:SER:CB	1:E:80:ILE:HD11	2.32	0.59
1:D:76:LEU:CD2	1:D:100:PRO:HD3	2.32	0.59
1:F:69:CYS:CB	1:F:101:CYS:HG	2.12	0.59
1:C:69:CYS:CB	1:C:101:CYS:HG	2.12	0.58
1:D:132:LEU:CD1	1:D:154:ILE:HG21	2.32	0.58
1:D:69:CYS:O	1:D:71:SER:N	2.35	0.58
1:D:20:PRO:HA	1:D:144:PHE:CD1	2.39	0.58
1:B:83:ILE:CD1	1:B:87:TYR:HA	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HG23	1:B:131:ARG:HB2	1.83	0.58
1:C:57:LEU:HB3	1:C:155:ILE:HG22	1.85	0.58
1:B:44:ARG:HB3	1:B:131:ARG:HH22	1.68	0.58
1:D:58:ILE:HG23	1:D:154:ILE:CG2	2.28	0.58
1:A:56:PHE:CD1	1:A:126:LEU:HD12	2.39	0.57
1:A:52:ILE:HA	1:A:128:LYS:HB2	1.86	0.57
1:F:69:CYS:HB3	1:F:101:CYS:SG	2.44	0.57
1:C:44:ARG:HH11	1:C:131:ARG:NH2	2.03	0.57
1:F:12:PRO:HD2	1:F:156:ALA:CB	2.34	0.57
1:B:94:LEU:HB3	1:B:120:LEU:HG	1.87	0.57
1:A:65:LYS:HG2	1:A:66:GLY:N	2.19	0.56
1:C:44:ARG:NH1	1:C:49:VAL:HG21	2.20	0.56
1:E:136:ILE:HD11	1:E:139:PRO:HA	1.88	0.56
1:F:44:ARG:HD3	1:F:131:ARG:HH12	1.71	0.56
1:E:69:CYS:O	1:E:71:SER:N	2.38	0.56
1:E:83:ILE:HD11	1:E:133:SER:OG	2.06	0.56
1:C:80:ILE:HA	1:C:133:SER:O	2.06	0.56
1:B:88:GLN:C	1:D:67:GLN:OE1	2.44	0.56
1:D:72:THR:O	1:D:73:HIS:CD2	2.58	0.56
1:C:65:LYS:HD3	1:C:66:GLY:N	2.21	0.56
1:E:79:THR:HG22	1:E:95:SER:OG	2.05	0.56
1:B:80:ILE:HD12	1:B:94:LEU:HD12	1.88	0.55
1:F:26:LEU:HD13	1:F:142:LEU:HD11	1.87	0.55
1:F:74:VAL:HB	2:F:266:HOH:O	2.07	0.55
1:F:36:LEU:O	1:F:37:LEU:HB2	2.07	0.55
1:D:69:CYS:CB	1:D:101:CYS:SG	2.95	0.55
1:E:51:PRO:O	1:E:128:LYS:HG3	2.07	0.55
1:A:29:SER:OG	1:A:31:ARG:HG2	2.06	0.55
1:C:52:ILE:HG12	1:C:53:GLU:H	1.72	0.54
1:B:61:GLN:HB3	1:B:151:TYR:CZ	2.42	0.54
1:C:70:PRO:O	1:C:71:SER:HB3	2.07	0.54
1:C:74:VAL:CG1	1:C:76:LEU:HD13	2.37	0.54
1:B:42:GLU:HB3	1:B:44:ARG:HH21	1.72	0.54
1:E:84:ALA:HB3	1:E:88:GLN:C	2.28	0.54
1:A:61:GLN:HB3	1:A:151:TYR:CZ	2.43	0.54
1:F:80:ILE:HD12	1:F:94:LEU:HD12	1.91	0.53
1:C:19:ASN:OD1	1:C:21:GLN:HB2	2.08	0.53
1:A:67:GLN:HG2	1:A:113:PRO:HB3	1.89	0.53
1:C:146:GLU:CD	1:D:72:THR:H	2.11	0.53
1:C:44:ARG:HD2	1:C:131:ARG:HH22	1.74	0.53
1:B:90:LYS:NZ	1:D:70:PRO:HG2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:HIS:CE1	1:C:102:GLN:O	2.62	0.53
1:A:51:PRO:O	1:A:128:LYS:HG3	2.09	0.53
1:D:79:THR:HG22	1:D:95:SER:OG	2.09	0.52
1:E:68:GLY:HA2	1:E:112:LYS:HD2	1.91	0.52
1:E:75:LEU:HD21	1:F:115:TYR:CE1	2.44	0.52
1:F:12:PRO:HD2	1:F:156:ALA:HB2	1.91	0.52
1:A:105:THR:H	1:A:106:PRO:HD2	1.75	0.52
1:B:69:CYS:O	1:B:71:SER:N	2.43	0.52
1:D:20:PRO:HA	1:D:144:PHE:HD1	1.74	0.52
1:F:15:HIS:HD1	1:F:59:TYR:HH	1.57	0.52
1:C:74:VAL:O	1:C:100:PRO:HD2	2.10	0.52
1:C:52:ILE:HG12	1:C:53:GLU:N	2.24	0.52
1:F:61:GLN:HA	1:F:118:ILE:O	2.10	0.51
1:D:11:LYS:HE2	1:D:156:ALA:O	2.11	0.51
1:D:69:CYS:HB3	1:D:101:CYS:SG	2.51	0.51
1:B:12:PRO:HA	1:B:39:ASN:HB2	1.92	0.51
1:E:64:PHE:HA	1:E:141:TYR:O	2.11	0.51
1:B:26:LEU:HD13	1:B:142:LEU:HD11	1.93	0.51
1:B:66:GLY:O	1:B:113:PRO:HA	2.10	0.51
1:C:69:CYS:CB	1:C:101:CYS:SG	2.98	0.51
1:C:14:ALA:CB	1:C:41:VAL:HG11	2.39	0.50
1:D:52:ILE:HG12	1:D:53:GLU:N	2.27	0.50
1:B:102:GLN:HG3	1:C:112:LYS:HD3	1.94	0.50
1:A:57:LEU:O	1:A:154:ILE:HA	2.12	0.50
1:B:112:LYS:H	1:B:112:LYS:HD2	1.77	0.50
1:A:31:ARG:HB3	1:A:31:ARG:CZ	2.41	0.50
1:B:65:LYS:HA	1:B:114:TRP:O	2.11	0.50
1:B:74:VAL:HG11	1:B:141:TYR:HE1	1.77	0.50
1:D:136:ILE:HD11	1:D:139:PRO:CA	2.41	0.50
1:C:57:LEU:O	1:C:154:ILE:HA	2.12	0.49
1:C:127:GLU:HG2	2:C:160:HOH:O	2.13	0.49
1:D:80:ILE:HA	1:D:133:SER:O	2.13	0.49
1:A:127:GLU:HB3	2:A:165:HOH:O	2.12	0.49
1:D:127:GLU:HG2	2:D:206:HOH:O	2.12	0.49
1:E:112:LYS:H	1:E:112:LYS:HD2	1.77	0.48
1:D:52:ILE:CG1	1:D:53:GLU:N	2.77	0.48
1:B:81:SER:HB3	2:B:164:HOH:O	2.12	0.48
1:E:12:PRO:HD2	1:E:156:ALA:HB3	1.95	0.48
1:C:136:ILE:CD1	1:C:142:LEU:HG	2.44	0.48
1:C:83:ILE:HG22	1:C:87:TYR:HA	1.95	0.48
1:F:50:VAL:HG23	1:F:130:ASP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HB2	1:A:157:LEU:HD11	1.96	0.48
1:A:80:ILE:HD12	1:A:94:LEU:HD12	1.96	0.48
1:D:142:LEU:HD13	1:D:144:PHE:HD2	1.79	0.48
1:A:70:PRO:O	1:A:71:SER:HB2	2.14	0.47
1:D:132:LEU:HD12	1:D:154:ILE:HG21	1.96	0.47
1:E:84:ALA:O	1:E:85:VAL:CG2	2.62	0.47
1:F:20:PRO:HA	1:F:144:PHE:CD1	2.50	0.47
1:E:118:ILE:HG22	1:E:120:LEU:HD13	1.95	0.47
1:B:83:ILE:HG13	1:B:88:GLN:O	2.14	0.47
1:D:70:PRO:O	1:D:71:SER:CB	2.51	0.47
1:E:72:THR:HG22	1:E:73:HIS:N	2.20	0.47
1:C:146:GLU:OE2	1:D:72:THR:CA	2.61	0.47
1:D:60:SER:HB3	1:D:80:ILE:HD11	1.97	0.47
1:F:142:LEU:HD13	1:F:144:PHE:CD2	2.50	0.47
1:E:77:THR:HG22	1:E:97:ILE:HG23	1.97	0.47
1:D:93:LEU:HB3	1:D:124:PHE:CZ	2.49	0.47
1:C:61:GLN:HA	1:C:118:ILE:O	2.15	0.47
1:E:75:LEU:HD22	1:E:97:ILE:HG22	1.97	0.47
1:A:77:THR:O	1:A:136:ILE:HA	2.14	0.47
1:D:98:LYS:HD3	1:D:116:GLU:HB3	1.97	0.47
1:E:70:PRO:O	1:E:71:SER:O	2.32	0.46
1:E:61:GLN:HB3	1:E:151:TYR:CZ	2.50	0.46
1:D:19:ASN:OD1	1:D:21:GLN:HB3	2.16	0.46
1:C:137:ASN:O	1:C:138:ARG:HD2	2.14	0.46
1:B:65:LYS:HG3	1:B:115:TYR:CE2	2.51	0.46
1:A:45:ASP:HB2	1:A:47:GLN:HE21	1.81	0.46
1:B:44:ARG:HD3	2:B:171:HOH:O	2.14	0.46
1:E:84:ALA:HB2	1:E:89:THR:O	2.16	0.46
1:E:79:THR:HG23	2:E:165:HOH:O	2.16	0.46
1:B:19:ASN:HD21	1:B:21:GLN:HB3	1.81	0.46
1:B:80:ILE:HA	1:B:133:SER:O	2.16	0.46
1:B:69:CYS:CB	1:B:101:CYS:SG	3.00	0.46
1:E:84:ALA:O	1:E:85:VAL:HG23	2.16	0.46
1:D:84:ALA:HA	1:D:130:ASP:OD1	2.16	0.46
1:A:104:GLU:O	1:A:105:THR:HG23	2.15	0.45
1:D:32:ARG:HH11	1:D:32:ARG:HG2	1.81	0.45
1:C:50:VAL:HG21	1:C:126:LEU:HD13	1.97	0.45
1:C:69:CYS:SG	1:C:101:CYS:CB	3.04	0.45
1:B:90:LYS:HB3	1:D:70:PRO:CG	2.46	0.45
1:B:69:CYS:HB3	1:B:101:CYS:SG	2.55	0.45
1:E:83:ILE:CB	1:E:131:ARG:HB2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:GLN:HA	1:E:139:PRO:HB2	1.99	0.45
1:E:35:ALA:O	1:E:36:LEU:HD23	2.16	0.45
1:A:72:THR:HG22	1:A:73:HIS:N	2.32	0.45
1:C:146:GLU:CD	1:D:72:THR:N	2.70	0.45
1:A:42:GLU:HG2	1:A:49:VAL:HB	1.99	0.45
1:E:84:ALA:HB3	1:E:88:GLN:O	2.17	0.44
1:C:68:GLY:C	1:C:70:PRO:HD3	2.38	0.44
1:F:28:TRP:CZ2	1:F:134:ALA:HB3	2.52	0.44
1:A:11:LYS:HA	1:A:12:PRO:HD3	1.85	0.44
1:B:105:THR:HA	1:B:106:PRO:HD2	1.93	0.44
1:A:136:ILE:HD13	1:A:142:LEU:HG	1.99	0.44
1:D:157:LEU:HD13	1:E:155:ILE:HG12	1.98	0.44
1:F:96:ALA:HB3	1:F:120:LEU:HD11	2.00	0.44
1:C:59:TYR:O	1:C:60:SER:HB2	2.17	0.44
1:A:64:PHE:HA	1:A:141:TYR:O	2.18	0.44
1:E:105:THR:OG1	1:E:106:PRO:HD2	2.18	0.44
1:F:83:ILE:HG12	1:F:131:ARG:CG	2.48	0.44
1:E:58:ILE:O	1:E:121:GLY:HA2	2.17	0.44
1:D:57:LEU:O	1:D:154:ILE:HA	2.18	0.44
1:E:56:PHE:CD1	1:E:126:LEU:HD12	2.53	0.44
1:F:110:GLU:O	1:F:111:ALA:HB3	2.18	0.44
1:A:103:ARG:O	1:A:104:GLU:HB2	2.18	0.43
1:C:49:VAL:HG22	1:C:131:ARG:HG2	1.99	0.43
1:D:82:ARG:NH2	1:D:130:ASP:OD2	2.51	0.43
1:A:53:GLU:HA	1:A:126:LEU:O	2.18	0.43
1:A:108:GLY:O	1:A:109:ALA:HB2	2.18	0.43
1:B:20:PRO:HA	1:B:144:PHE:CD1	2.53	0.43
1:A:94:LEU:HD13	1:A:121:GLY:N	2.33	0.43
1:E:75:LEU:HD21	1:F:115:TYR:CD1	2.54	0.43
1:E:60:SER:HB2	1:E:80:ILE:HD11	1.99	0.43
1:E:74:VAL:HG11	1:E:141:TYR:CE1	2.54	0.43
1:E:53:GLU:HG2	1:E:54:GLY:H	1.84	0.43
1:B:133:SER:HB2	2:B:208:HOH:O	2.18	0.43
1:B:67:GLN:OE1	1:B:113:PRO:HB3	2.19	0.43
1:F:57:LEU:O	1:F:154:ILE:HA	2.19	0.43
1:C:146:GLU:CB	1:D:71:SER:HB3	2.47	0.43
1:F:12:PRO:HB3	1:F:51:PRO:HG3	2.01	0.42
1:F:13:VAL:CG2	1:F:36:LEU:HD13	2.49	0.42
1:A:20:PRO:HA	1:A:144:PHE:CD1	2.54	0.42
1:C:12:PRO:HA	1:C:39:ASN:HB2	2.00	0.42
1:B:90:LYS:HB3	1:D:70:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HB3	1:A:150:VAL:HG21	2.00	0.42
1:E:65:LYS:HG2	1:E:66:GLY:N	2.35	0.42
1:A:69:CYS:CB	1:A:101:CYS:SG	3.07	0.42
1:F:20:PRO:HA	1:F:144:PHE:CE1	2.55	0.42
1:A:72:THR:CG2	1:A:73:HIS:N	2.83	0.42
1:A:60:SER:OG	1:A:78:HIS:CE1	2.73	0.42
1:B:109:ALA:HB1	1:B:112:LYS:HE3	2.02	0.42
1:B:127:GLU:O	1:B:130:ASP:HB2	2.20	0.42
1:C:69:CYS:HB3	1:C:101:CYS:HB3	2.01	0.42
1:A:93:LEU:HD22	1:A:124:PHE:CD2	2.55	0.42
1:E:102:GLN:OE1	1:E:102:GLN:HA	2.20	0.42
1:C:84:ALA:HA	1:C:130:ASP:OD1	2.20	0.42
1:F:83:ILE:HG12	1:F:131:ARG:HG2	2.02	0.41
1:D:79:THR:HG23	2:D:178:HOH:O	2.20	0.41
1:E:105:THR:CB	1:E:106:PRO:CD	2.98	0.41
1:D:71:SER:O	1:D:72:THR:O	2.37	0.41
1:D:65:LYS:HA	1:D:114:TRP:O	2.19	0.41
1:F:62:VAL:HG11	1:F:136:ILE:CG2	2.50	0.41
1:B:44:ARG:O	1:B:131:ARG:NH2	2.53	0.41
1:D:112:LYS:HB3	2:F:1579:HOH:O	2.20	0.41
1:A:21:GLN:O	1:A:22:ALA:C	2.59	0.41
1:E:50:VAL:HA	1:E:51:PRO:HD2	1.86	0.41
1:C:85:VAL:HG12	1:C:86:SER:N	2.35	0.41
1:A:114:TRP:HB3	1:C:102:GLN:NE2	2.36	0.41
1:E:136:ILE:CD1	1:E:139:PRO:HA	2.49	0.41
1:E:118:ILE:HG21	1:E:118:ILE:HD13	1.77	0.41
1:D:33:ALA:HB3	2:D:162:HOH:O	2.19	0.41
1:A:20:PRO:HA	1:A:144:PHE:HD1	1.86	0.41
1:C:76:LEU:HA	1:C:76:LEU:HD12	1.92	0.41
1:F:10:ASP:HA	1:F:39:ASN:OD1	2.21	0.41
1:E:76:LEU:HD22	1:E:100:PRO:HD3	2.03	0.41
1:A:148:GLY:HA2	2:A:160:HOH:O	2.22	0.40
1:E:33:ALA:O	1:E:34:ASN:HB2	2.21	0.40
1:F:49:VAL:HG12	2:F:217:HOH:O	2.21	0.40
1:B:58:ILE:O	1:B:121:GLY:HA2	2.21	0.40
1:E:61:GLN:HA	1:E:118:ILE:O	2.21	0.40
1:D:108:GLY:O	1:D:109:ALA:HB3	2.20	0.40
1:C:11:LYS:HA	1:C:12:PRO:HD3	1.89	0.40

All (6) 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:A:177:HOH:O	2:F:192:HOH:H1[4_555]	1.20	0.40
2:A:177:HOH:H1	2:F:192:HOH:H1[4_555]	1.30	0.30
1:B:53:GLU:O	1:E:31:ARG:NH2[4_455]	2.05	0.15
2:A:180:HOH:H1	2:F:1578:HOH:O[4_555]	1.47	0.13
2:A:177:HOH:O	2:F:192:HOH:O[4_555]	2.08	0.12
2:A:180:HOH:O	2:F:1578:HOH:O[4_555]	2.17	0.03

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	147/150 (98%)	120 (82%)	15 (10%)	12 (8%)	1	1
1	B	147/150 (98%)	128 (87%)	14 (10%)	5 (3%)	5	6
1	C	147/150 (98%)	126 (86%)	13 (9%)	8 (5%)	2	2
1	D	147/150 (98%)	124 (84%)	17 (12%)	6 (4%)	3	4
1	E	147/150 (98%)	128 (87%)	11 (8%)	8 (5%)	2	2
1	F	147/150 (98%)	124 (84%)	16 (11%)	7 (5%)	3	3
All	All	882/900 (98%)	750 (85%)	86 (10%)	46 (5%)	2	2

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	B	111	ALA
1	C	104	GLU
1	D	72	THR
1	D	86	SER
1	E	72	THR
1	E	84	ALA
1	E	105	THR
1	F	37	LEU
1	F	85	VAL

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Mol	Chain	Res	Type
1	A	85	VAL
1	A	105	THR
1	A	109	ALA
1	A	147	SER
1	B	70	PRO
1	B	85	VAL
1	B	86	SER
1	C	85	VAL
1	C	105	THR
1	D	70	PRO
1	D	109	ALA
1	E	70	PRO
1	E	85	VAL
1	E	104	GLU
1	F	72	THR
1	A	72	THR
1	B	72	THR
1	C	71	SER
1	C	107	GLU
1	D	110	GLU
1	E	37	LEU
1	F	147	SER
1	A	37	LEU
1	A	70	PRO
1	A	112	LYS
1	C	72	THR
1	F	111	ALA
1	A	23	GLU
1	A	87	TYR
1	A	108	GLY
1	C	37	LEU
1	D	85	VAL
1	E	87	TYR
1	F	107	GLU
1	C	70	PRO
1	F	106	PRO

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	116/126 (92%)	107 (92%)	9 (8%)	16	29
1	B	114/126 (90%)	106 (93%)	8 (7%)	19	34
1	C	115/126 (91%)	101 (88%)	14 (12%)	6	11
1	D	114/126 (90%)	103 (90%)	11 (10%)	10	19
1	E	114/126 (90%)	102 (90%)	12 (10%)	8	16
1	F	114/126 (90%)	105 (92%)	9 (8%)	15	28
All	All	687/756 (91%)	624 (91%)	63 (9%)	11	21

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	53	GLU
1	A	76	LEU
1	A	79	THR
1	A	83	ILE
1	A	112	LYS
1	A	120	LEU
1	A	133	SER
1	A	142	LEU
1	B	12	PRO
1	B	21	GLN
1	B	69	CYS
1	B	76	LEU
1	B	89	THR
1	B	112	LYS
1	B	120	LEU
1	B	142	LEU
1	C	32	ARG
1	C	42	GLU
1	C	43	LEU
1	C	44	ARG
1	C	45	ASP
1	C	75	LEU
1	C	76	LEU
1	C	105	THR
1	C	112	LYS
1	C	120	LEU

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Mol	Chain	Res	Type
1	C	135	GLU
1	C	142	LEU
1	C	144	PHE
1	C	155	ILE
1	D	21	GLN
1	D	31	ARG
1	D	43	LEU
1	D	44	ARG
1	D	53	GLU
1	D	67	GLN
1	D	76	LEU
1	D	100	PRO
1	D	112	LYS
1	D	120	LEU
1	D	142	LEU
1	E	21	GLN
1	E	43	LEU
1	E	44	ARG
1	E	53	GLU
1	E	75	LEU
1	E	76	LEU
1	E	82	ARG
1	E	112	LYS
1	E	120	LEU
1	E	131	ARG
1	E	142	LEU
1	E	144	PHE
1	F	21	GLN
1	F	43	LEU
1	F	53	GLU
1	F	69	CYS
1	F	76	LEU
1	F	83	ILE
1	F	102	GLN
1	F	105	THR
1	F	142	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	47	GLN

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Mol	Chain	Res	Type
1	A	73	HIS
1	A	78	HIS
1	A	125	GLN
1	A	149	GLN
1	B	21	GLN
1	B	73	HIS
1	B	149	GLN
1	D	73	HIS
1	D	78	HIS
1	D	92	ASN
1	D	149	GLN
1	E	47	GLN
1	E	73	HIS
1	F	47	GLN
1	F	102	GLN
1	F	125	GLN
1	F	149	GLN

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 (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	149/150 (99%)	0.54	12 (8%)	15	16	7, 17, 66, 78	0
1	B	149/150 (99%)	0.38	13 (8%)	13	13	7, 16, 65, 74	0
1	C	149/150 (99%)	0.63	16 (10%)	8	8	7, 18, 62, 74	0
1	D	149/150 (99%)	0.72	9 (6%)	25	28	8, 17, 59, 75	0
1	E	149/150 (99%)	1.11	24 (16%)	3	2	7, 17, 62, 68	0
1	F	149/150 (99%)	1.28	30 (20%)	1	1	7, 19, 69, 79	0
All	All	894/900 (99%)	0.78	104 (11%)	6	6	7, 18, 64, 79	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	11.1
1	A	86	SER	7.9
1	D	86	SER	7.8
1	A	108	GLY	7.6
1	D	105	THR	7.4
1	B	86	SER	7.3
1	C	106	PRO	7.3
1	E	85	VAL	7.2
1	F	109	ALA	7.1
1	A	105	THR	7.0
1	B	108	GLY	5.9
1	C	70	PRO	5.8
1	B	109	ALA	5.8
1	C	86	SER	5.7
1	D	87	TYR	5.3
1	F	108	GLY	5.0
1	F	107	GLU	5.0
1	F	87	TYR	5.0
1	D	72	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	105	THR	5.0
1	D	107	GLU	4.9
1	E	106	PRO	4.9
1	C	105	THR	4.7
1	A	106	PRO	4.5
1	B	72	THR	4.5
1	C	74	VAL	4.4
1	C	72	THR	4.4
1	A	110	GLU	4.2
1	F	86	SER	4.2
1	C	107	GLU	4.2
1	D	111	ALA	4.1
1	B	103	ARG	4.0
1	D	106	PRO	3.9
1	F	44	ARG	3.9
1	C	108	GLY	3.9
1	E	87	TYR	3.9
1	A	72	THR	3.8
1	F	103	ARG	3.8
1	E	70	PRO	3.8
1	E	108	GLY	3.7
1	F	70	PRO	3.7
1	E	74	VAL	3.7
1	C	24	GLY	3.7
1	C	22	ALA	3.6
1	F	85	VAL	3.5
1	E	22	ALA	3.5
1	A	107	GLU	3.5
1	F	22	ALA	3.5
1	E	109	ALA	3.5
1	E	72	THR	3.4
1	C	73	HIS	3.4
1	B	110	GLU	3.4
1	C	109	ALA	3.4
1	A	85	VAL	3.3
1	E	75	LEU	3.2
1	C	87	TYR	3.2
1	B	111	ALA	3.2
1	E	9	SER	3.2
1	E	86	SER	3.1
1	E	131	ARG	3.1
1	F	146	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	40	GLY	2.9
1	E	110	GLU	2.9
1	A	87	TYR	2.9
1	A	52	ILE	2.9
1	F	71	SER	2.8
1	B	71	SER	2.8
1	D	9	SER	2.7
1	B	102	GLN	2.7
1	E	67	GLN	2.7
1	F	104	GLU	2.7
1	B	9	SER	2.7
1	E	89	THR	2.7
1	D	56	PHE	2.6
1	E	68	GLY	2.6
1	F	105	THR	2.6
1	A	71	SER	2.5
1	E	107	GLU	2.5
1	C	71	SER	2.5
1	F	12	PRO	2.4
1	F	69	CYS	2.4
1	F	67	GLN	2.4
1	E	23	GLU	2.4
1	F	48	LEU	2.3
1	F	9	SER	2.3
1	E	41	VAL	2.3
1	F	150	VAL	2.3
1	B	100	PRO	2.3
1	F	36	LEU	2.2
1	E	53	GLU	2.2
1	F	72	THR	2.2
1	C	110	GLU	2.1
1	E	44	ARG	2.1
1	F	18	ALA	2.1
1	E	104	GLU	2.1
1	F	39	ASN	2.1
1	B	101	CYS	2.1
1	F	17	VAL	2.0
1	F	80	ILE	2.0
1	F	38	ALA	2.0
1	B	106	PRO	2.0
1	F	106	PRO	2.0
1	C	9	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	34	ASN	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.