Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 10:53 AM EDT

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)

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 ⓘ) were used in the production of this report:

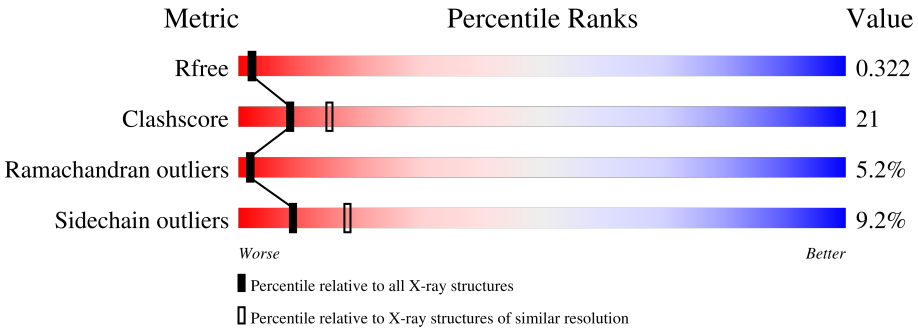
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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%

Mol	Chain	Length	Quality of chain
1	A	150	53% 37% 8% ••
1	B	150	63% 30% 7% •
1	C	150	53% 39% 7% ••
1	D	150	60% 31% 7% ••
1	E	150	52% 38% 8% ••
1	F	150	59% 36% • ••

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 mutation	UNP P01375
A	52	ILE	SER	engineered mutation	UNP P01375
A	56	PHE	TYR	engineered mutation	UNP P01375
B	29	SER	LEU	engineered mutation	UNP P01375
B	52	ILE	SER	engineered mutation	UNP P01375
B	56	PHE	TYR	engineered mutation	UNP P01375
C	29	SER	LEU	engineered mutation	UNP P01375
C	52	ILE	SER	engineered mutation	UNP P01375
C	56	PHE	TYR	engineered mutation	UNP P01375
D	29	SER	LEU	engineered mutation	UNP P01375
D	52	ILE	SER	engineered mutation	UNP P01375
D	56	PHE	TYR	engineered mutation	UNP P01375
E	29	SER	LEU	engineered mutation	UNP P01375
E	52	ILE	SER	engineered mutation	UNP P01375
E	56	PHE	TYR	engineered mutation	UNP P01375
F	29	SER	LEU	engineered mutation	UNP P01375
F	52	ILE	SER	engineered mutation	UNP P01375

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

- Molecule 2 is water.

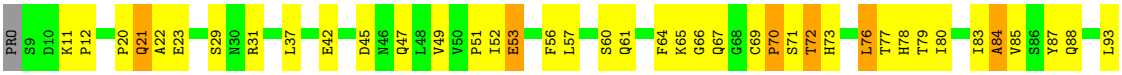
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	57	Total	H	O	0	0
			171	114	57		
2	B	66	Total	H	O	0	0
			198	132	66		
2	C	55	Total	H	O	0	0
			165	110	55		
2	D	62	Total	H	O	0	0
			186	124	62		
2	E	58	Total	H	O	0	0
			174	116	58		
2	F	58	Total	H	O	0	0
			174	116	58		

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. 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. 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.

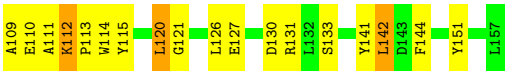
• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain A:



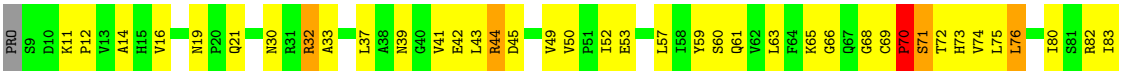
• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain B:



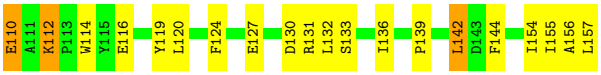
• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain C:



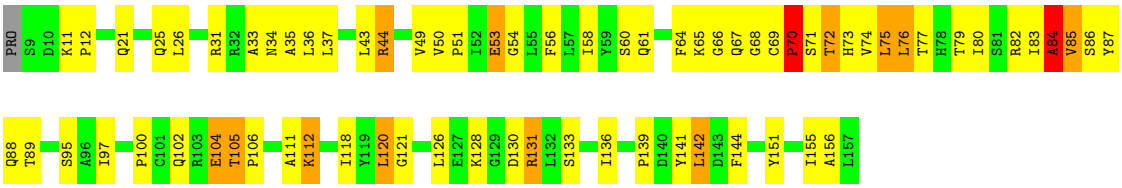
• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain D:



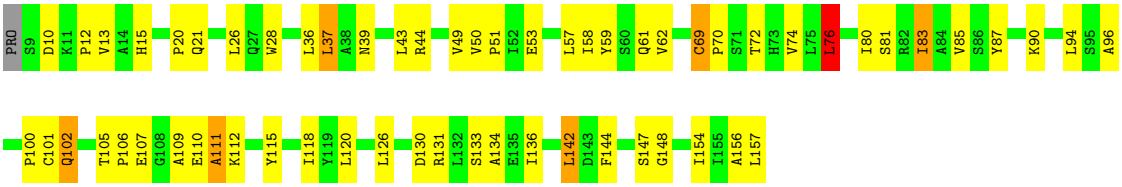
• Molecule 1: PROTEIN (TUMOR NECROSIS FACTOR-ALPHA)

Chain E:



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

Chain F:



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 0.327 , 0.322	Depositor DCC
R_{free} test set	8150 reflections (20.16%)	wwPDB-VP
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 , 111.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
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
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.*

[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	0.65	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(^{o})	Ideal(^{o})
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	45	1
1	C	1122	245	1108	52	0
1	D	1118	245	1103	58	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	275	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 (275) 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:C:69:CYS:SG	1:C:101:CYS:SG	2.47	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:D:69:CYS:SG	1:D:101:CYS:SG	2.54	0.92
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:B:69:CYS:SG	1:B:101:CYS:SG	2.59	0.88
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:D:76:LEU:HD22	1:D:100:PRO:HD3	1.71	0.71
1:E:50:VAL:HG21	1:E:126:LEU:HD13	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:66:GLY:O	1:A:113:PRO:HA	1.93	0.68
1:F:76:LEU:HD22	1:F:100:PRO:HD3	1.75	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:32:ARG:HD3	1:C:33:ALA:N	2.10	0.66
1:C:146:GLU:OE2	1:D:72:THR:HA	1.96	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:C:16:VAL:HG12	1:C:30:ASN:HB3	1.80	0.63
1:E:80:ILE:HA	1:E:133:SER:O	1.98	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:32:ARG:HD3	1:C:33:ALA:H	1.65	0.61
1:C:146:GLU:OE2	1:D:72:THR:N	2.33	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:B:58:ILE:HD11	1:B:126:LEU:HD11	1.82	0.61
1:F:109:ALA:HB1	1:F:112:LYS:HE2	1.83	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:D:76:LEU:CD2	1:D:100:PRO:HD3	2.32	0.59
1:E:60:SER:CB	1:E:80:ILE:HD11	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:69:CYS:O	1:D:71:SER:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:CD1	1:D:154:ILE:HG21	2.32	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
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:E:69:CYS:O	1:E:71:SER:N	2.38	0.56
1:F:44:ARG:HD3	1:F:131:ARG:HH12	1.71	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:C:65:LYS:HD3	1:C:66:GLY:N	2.21	0.56
1:D:72:THR:O	1:D:73:HIS:CD2	2.58	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:36:LEU:O	1:F:37:LEU:HB2	2.07	0.55
1:F:74:VAL:HB	2:F:266:HOH:O	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:B:61:GLN:HB3	1:B:151:TYR:CZ	2.42	0.54
1:C:52:ILE:HG12	1:C:53:GLU:H	1.72	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:C:19:ASN:OD1	1:C:21:GLN:HB2	2.08	0.53
1:F:80:ILE:HD12	1:F:94:LEU:HD12	1.91	0.53
1:A:67:GLN:HG2	1:A:113:PRO:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ARG:HD2	1:C:131:ARG:HH22	1.74	0.53
1:C:146:GLU:CD	1:D:72:THR:H	2.11	0.53
1:A:51:PRO:O	1:A:128:LYS:HG3	2.09	0.53
1:B:90:LYS:NZ	1:D:70:PRO:HG2	2.23	0.53
1:C:73:HIS:CE1	1:C:102:GLN:O	2.62	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:D:11:LYS:HE2	1:D:156:ALA:O	2.11	0.51
1:F:61:GLN:HA	1:F:118:ILE:O	2.10	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: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:E:64:PHE:HA	1:E:141:TYR:O	2.11	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:HD2	1:E:112:LYS:H	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:C:136:ILE:CD1	1:C:142:LEU:HG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:PRO:HD2	1:E:156:ALA:HB3	1.95	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
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:E:118:ILE:HG22	1:E:120:LEU:HD13	1.95	0.47
1:F:20:PRO:HA	1:F:144:PHE:CD1	2.50	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:C:61:GLN:HA	1:C:118:ILE:O	2.15	0.47
1:D:93:LEU:HB3	1:D:124:PHE:CZ	2.49	0.47
1:E:77:THR:HG22	1:E:97:ILE:HG23	1.97	0.47
1:A:77:THR:O	1:A:136:ILE:HA	2.14	0.47
1:E:75:LEU:HD22	1:E:97:ILE:HG22	1.97	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:D:19:ASN:OD1	1:D:21:GLN:HB3	2.16	0.46
1:E:61:GLN:HB3	1:E:151:TYR:CZ	2.50	0.46
1:C:137:ASN:O	1:C:138:ARG:HD2	2.14	0.46
1:A:45:ASP:HB2	1:A:47:GLN:HE21	1.81	0.46
1:B:65:LYS:HG3	1:B:115:TYR:CE2	2.51	0.46
1:B:19:ASN:HD21	1:B:21:GLN:HB3	1.81	0.46
1:B:44:ARG:HD3	2:B:171:HOH:O	2.14	0.46
1:E:79:THR:HG23	2:E:165:HOH:O	2.16	0.46
1:E:84:ALA:HB2	1:E:89:THR:O	2.16	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:D:84:ALA:HA	1:D:130:ASP:OD1	2.16	0.46
1:E:84:ALA:O	1:E:85:VAL:HG23	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:B:90:LYS:HB3	1:D:70:PRO:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:CYS:SG	1:C:101:CYS:CB	3.04	0.45
1:B:69:CYS:HB3	1:B:101:CYS:SG	2.55	0.45
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:E:83:ILE:CB	1:E:131:ARG:HB2	2.43	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:A:11:LYS:HA	1:A:12:PRO:HD3	1.85	0.44
1:C:68:GLY:C	1:C:70:PRO:HD3	2.38	0.44
1:E:84:ALA:HB3	1:E:88:GLN:O	2.17	0.44
1:F:28:TRP:CZ2	1:F:134:ALA:HB3	2.52	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:A:64:PHE:HA	1:A:141:TYR:O	2.18	0.44
1:C:59:TYR:O	1:C:60:SER:HB2	2.17	0.44
1:E:105:THR:OG1	1:E:106:PRO:HD2	2.18	0.44
1:F:96:ALA:HB3	1:F:120:LEU:HD11	2.00	0.44
1:E:58:ILE:O	1:E:121:GLY:HA2	2.17	0.44
1:F:83:ILE:HG12	1:F:131:ARG:CG	2.48	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:B:67:GLN:OE1	1:B:113:PRO:HB3	2.19	0.43
1:B:133:SER:HB2	2:B:208:HOH:O	2.18	0.43
1:E:53:GLU:HG2	1:E:54:GLY:H	1.84	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: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:A:20:PRO:HA	1:A:144:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:CG2	1:F:36:LEU:HD13	2.49	0.42
1:C:12:PRO:HA	1:C:39:ASN:HB2	2.00	0.42
1:A:144:PHE:HB3	1:A:150:VAL:HG21	2.00	0.42
1:B:90:LYS:HB3	1:D:70:PRO:HG2	2.01	0.42
1:E:65:LYS:HG2	1:E:66:GLY:N	2.35	0.42
1:A:60:SER:OG	1:A:78:HIS:CE1	2.73	0.42
1:A:69:CYS:CB	1:A:101:CYS:SG	3.07	0.42
1:A:72:THR:CG2	1:A:73:HIS:N	2.83	0.42
1:F:20:PRO:HA	1:F:144:PHE:CE1	2.55	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:A:93:LEU:HD22	1:A:124:PHE:CD2	2.55	0.42
1:C:69:CYS:HB3	1:C:101:CYS:HB3	2.01	0.42
1:C:84:ALA:HA	1:C:130:ASP:OD1	2.20	0.42
1:E:102:GLN:OE1	1:E:102:GLN:HA	2.20	0.42
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:F:83:ILE:HG12	1:F:131:ARG:HG2	2.02	0.41
1:D:65:LYS:HA	1:D:114:TRP:O	2.19	0.41
1:D:71:SER:O	1:D:72:THR:O	2.37	0.41
1:F:62:VAL:HG11	1:F:136:ILE:CG2	2.50	0.41
1:A:21:GLN:O	1:A:22:ALA:C	2.59	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:C:85:VAL:HG12	1:C:86:SER:N	2.35	0.41
1:E:50:VAL:HA	1:E:51:PRO:HD2	1.86	0.41
1:A:114:TRP:HB3	1:C:102:GLN:NE2	2.36	0.41
1:D:33:ALA:HB3	2:D:162:HOH:O	2.19	0.41
1:E:118:ILE:HG21	1:E:118:ILE:HD13	1.77	0.41
1:E:136:ILE:CD1	1:E:139:PRO:HA	2.49	0.41
1:A:20:PRO:HA	1:A:144:PHE:HD1	1.86	0.41
1:C:76:LEU:HD12	1:C:76:LEU:HA	1.92	0.41
1:E:76:LEU:HD22	1:E:100:PRO:HD3	2.03	0.41
1:F:10:ASP:HA	1:F:39:ASN:OD1	2.21	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:D:108:GLY:O	1:D:109:ALA:HB3	2.20	0.40
1:E:61:GLN:HA	1:E:118:ILE:O	2.21	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%)	3	5
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	3
1	E	147/150 (98%)	128 (87%)	11 (8%)	8 (5%)	2	2
1	F	147/150 (98%)	124 (84%)	16 (11%)	7 (5%)	2	2
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

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Mol	Chain	Res	Type
1	E	105	THR
1	F	37	LEU
1	F	85	VAL
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%)	12 24
1	B	114/126 (90%)	106 (93%)	8 (7%)	15 29
1	C	115/126 (91%)	101 (88%)	14 (12%)	5 9
1	D	114/126 (90%)	103 (90%)	11 (10%)	8 16
1	E	114/126 (90%)	102 (90%)	12 (10%)	7 13
1	F	114/126 (90%)	105 (92%)	9 (8%)	12 24
All	All	687/756 (91%)	624 (91%)	63 (9%)	9 18

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

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Mol	Chain	Res	Type
1	C	75	LEU
1	C	76	LEU
1	C	105	THR
1	C	112	LYS
1	C	120	LEU
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

Sometimes 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
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

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2
1	C	1
1	B	1
1	D	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	88:GLN	C	89:THR	N	1.19
1	B	110:GLU	C	111:ALA	N	1.18
1	E	70:PRO	C	71:SER	N	1.16
1	D	70:PRO	C	71:SER	N	1.13
1	A	88:GLN	C	89:THR	N	1.11
1	E	84:ALA	C	85:VAL	N	1.05

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.