Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:53 PM GMT

PDB ID	:	4ATZ
Title	:	Ad5 knob in complex with a designed ankyrin repeat protein
Authors	:	Mittl, P.R.E.; Hess, C.; Dreier, B.
Deposited on	:	2012-05-11
Resolution	:	1.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

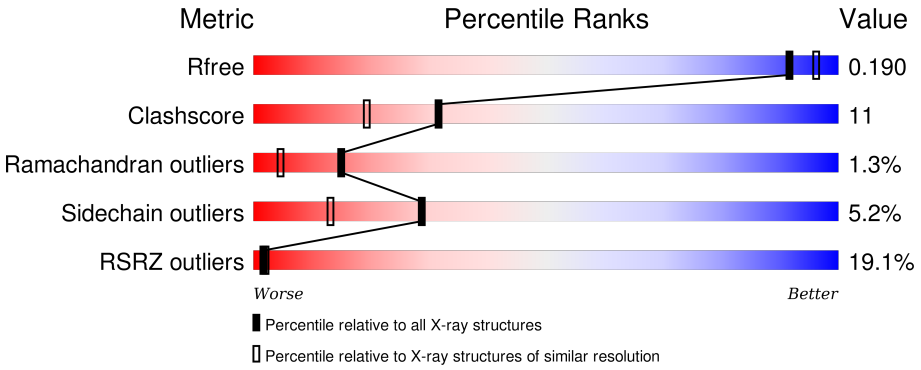
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	201	11% 69% 17% 9%
1	B	201	14% 67% 16% 15%
1	C	201	15% 72% 12% 12%
2	D	154	10% 77% 20%
2	E	154	16% 83% 15%

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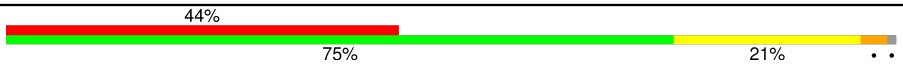
Mol	Chain	Length	Quality of chain
2	F	154	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8492 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 FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	14	0
			1499	949	250	296	4			
1	B	171	Total	C	N	O	S	0	11	0
			1402	892	233	273	4			
1	C	176	Total	C	N	O	S	0	3	0
			1374	873	226	271	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	MET	-	EXPRESSION TAG	UNP P11818
A	382	ALA	-	EXPRESSION TAG	UNP P11818
A	383	HIS	-	EXPRESSION TAG	UNP P11818
A	384	HIS	-	EXPRESSION TAG	UNP P11818
A	385	HIS	-	EXPRESSION TAG	UNP P11818
A	386	HIS	-	EXPRESSION TAG	UNP P11818
A	387	HIS	-	EXPRESSION TAG	UNP P11818
A	388	HIS	-	EXPRESSION TAG	UNP P11818
A	389	GLY	-	EXPRESSION TAG	UNP P11818
A	390	SER	-	EXPRESSION TAG	UNP P11818
A	.	-	THR	DELETION	UNP P11818
A	.	-	ALA	DELETION	UNP P11818
A	.	-	TYR	DELETION	UNP P11818
A	.	-	THR	DELETION	UNP P11818
B	377	MET	-	EXPRESSION TAG	UNP P11818
B	378	ALA	-	EXPRESSION TAG	UNP P11818
B	379	HIS	-	EXPRESSION TAG	UNP P11818
B	380	HIS	-	EXPRESSION TAG	UNP P11818
B	381	HIS	-	EXPRESSION TAG	UNP P11818
B	382	HIS	-	EXPRESSION TAG	UNP P11818
B	383	HIS	-	EXPRESSION TAG	UNP P11818
B	384	HIS	-	EXPRESSION TAG	UNP P11818
B	385	GLY	-	EXPRESSION TAG	UNP P11818

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Chain	Residue	Modelled	Actual	Comment	Reference
B	386	SER	-	EXPRESSION TAG	UNP P11818
B	.	-	THR	DELETION	UNP P11818
B	.	-	ALA	DELETION	UNP P11818
B	.	-	TYR	DELETION	UNP P11818
B	.	-	THR	DELETION	UNP P11818
C	377	MET	-	EXPRESSION TAG	UNP P11818
C	378	ALA	-	EXPRESSION TAG	UNP P11818
C	379	HIS	-	EXPRESSION TAG	UNP P11818
C	380	HIS	-	EXPRESSION TAG	UNP P11818
C	381	HIS	-	EXPRESSION TAG	UNP P11818
C	382	HIS	-	EXPRESSION TAG	UNP P11818
C	383	HIS	-	EXPRESSION TAG	UNP P11818
C	384	HIS	-	EXPRESSION TAG	UNP P11818
C	385	GLY	-	EXPRESSION TAG	UNP P11818
C	386	SER	-	EXPRESSION TAG	UNP P11818
C	.	-	THR	DELETION	UNP P11818
C	.	-	ALA	DELETION	UNP P11818
C	.	-	TYR	DELETION	UNP P11818
C	.	-	THR	DELETION	UNP P11818

- Molecule 2 is a protein called DESIGNED ANKYRIN REPEAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	0	2	0
			1172	742	200	228	2			
2	E	154	Total	C	N	O	S	0	1	0
			1167	739	199	227	2			
2	F	152	Total	C	N	O	S	0	0	0
			1143	721	197	223	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	178	Total	O	0	0
			178	178		
3	C	132	Total	O	0	0
			132	132		
3	D	102	Total	O	0	0
			102	102		
3	E	74	Total	O	0	0
			74	74		

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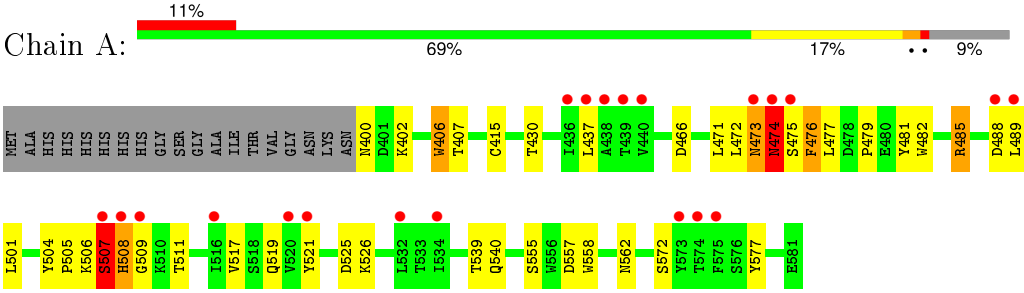
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	48	Total O 48 48	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

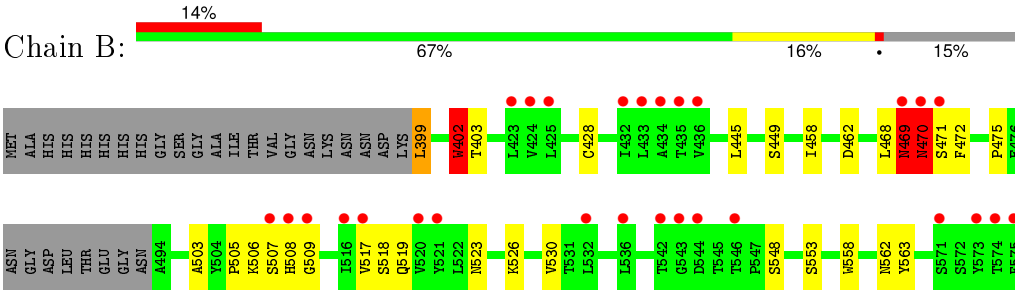
- Molecule 1: FIBER PROTEIN

Chain A:



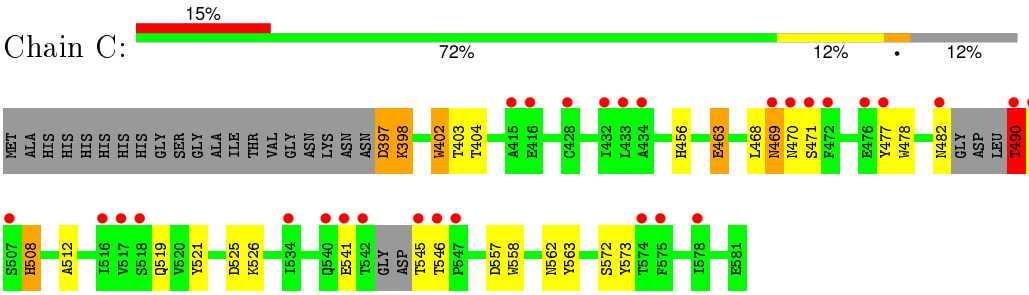
- Molecule 1: FIBER PROTEIN

Chain B:



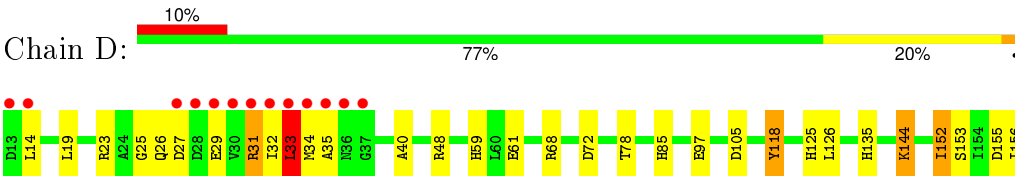
- Molecule 1: FIBER PROTEIN

Chain C:



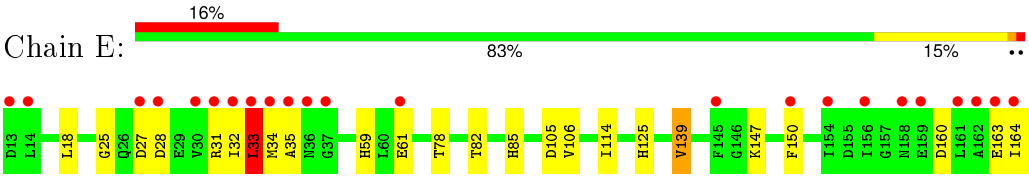
- Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN

Chain D:



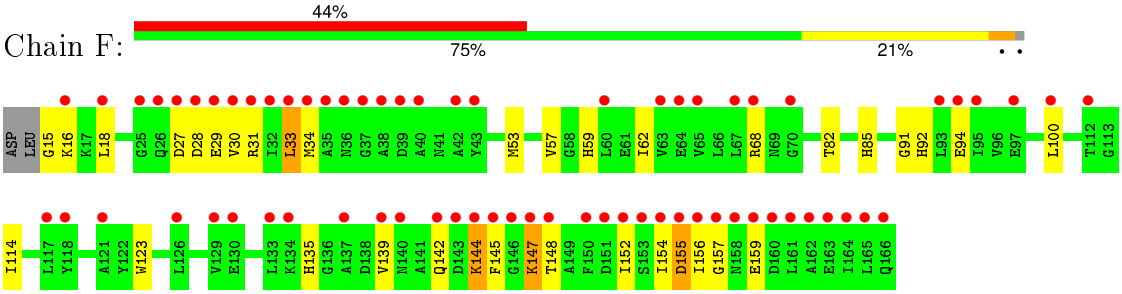
• Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN

Chain E:



• Molecule 2: DESIGNED ANKYRIN REPEAT PROTEIN

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	109.60Å 112.10Å 129.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 1.95 46.57 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.57-1.95) 100.0 (46.57-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.161 , 0.193 0.157 , 0.190	Depositor DCC
R_{free} test set	5802 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.9	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 116677 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8492	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.51	10/1540 (0.6%)	1.31	6/2096 (0.3%)
1	B	1.48	7/1439 (0.5%)	1.24	6/1959 (0.3%)
1	C	1.37	8/1411 (0.6%)	1.19	3/1922 (0.2%)
2	D	1.24	2/1193 (0.2%)	1.09	8/1623 (0.5%)
2	E	1.10	0/1189	1.04	4/1617 (0.2%)
2	F	0.94	1/1161 (0.1%)	0.86	0/1579
All	All	1.31	28/7933 (0.4%)	1.15	27/10796 (0.3%)

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	3
1	B	0	1
1	C	0	2
All	All	0	6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	TRP	CD2-CE2	7.91	1.50	1.41
1	B	518	SER	CB-OG	7.88	1.52	1.42
1	A	504	TYR	CD1-CE1	6.92	1.49	1.39
1	A	485	ARG	CZ-NH1	6.87	1.42	1.33
2	F	123	TRP	CD2-CE2	6.63	1.49	1.41
1	C	402	TRP	CD2-CE2	6.39	1.49	1.41
1	A	558	TRP	CD2-CE2	6.23	1.48	1.41
1	C	573	TYR	CG-CD1	6.11	1.47	1.39
1	C	463	GLU	CG-CD	5.94	1.60	1.51
1	A	555	SER	CB-OG	5.88	1.49	1.42
2	D	118	TYR	CG-CD1	5.70	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	563	TYR	CG-CD2	5.67	1.46	1.39
1	A	482	TRP	CG-CD1	5.62	1.44	1.36
2	D	118	TYR	CE2-CZ	5.57	1.45	1.38
1	C	573	TYR	CG-CD2	5.51	1.46	1.39
1	C	478	TRP	CD2-CE2	5.45	1.47	1.41
1	B	558	TRP	CB-CG	5.31	1.59	1.50
1	A	406	TRP	CG-CD1	5.30	1.44	1.36
1	A	558	TRP	CG-CD1	5.25	1.44	1.36
1	B	449	SER	CB-OG	5.20	1.49	1.42
1	B	478	TRP	CD2-CE2	5.20	1.47	1.41
1	C	572	SER	CB-OG	5.19	1.49	1.42
1	B	563	TYR	CE1-CZ	5.18	1.45	1.38
1	A	577	TYR	CD1-CE1	5.14	1.47	1.39
1	B	563	TYR	CG-CD2	5.06	1.45	1.39
1	C	558	TRP	CD2-CE2	5.05	1.47	1.41
1	A	493	ASN	C-O	5.02	1.32	1.23
1	A	572	SER	CA-CB	5.00	1.60	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	485	ARG	NE-CZ-NH2	-11.47	114.57	120.30
1	A	466	ASP	CB-CG-OD1	7.85	125.36	118.30
1	B	399	LEU	CB-CG-CD2	-6.84	99.37	111.00
2	D	105	ASP	CB-CG-OD1	6.56	124.21	118.30
1	B	399	LEU	CB-CG-CD1	6.54	122.11	111.00
2	D	33	LEU	CA-CB-CG	6.49	130.24	115.30
1	B	462	ASP	CB-CG-OD1	6.37	124.03	118.30
2	E	33	LEU	CA-CB-CG	6.35	129.90	115.30
2	E	105	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	525	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	501	LEU	CB-CG-CD1	-6.21	100.45	111.00
2	E	139	VAL	CB-CA-C	-6.15	99.71	111.40
2	D	72	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	525	ASP	CB-CG-OD1	5.87	123.58	118.30
2	D	152	ILE	CG1-CB-CG2	5.61	123.74	111.40
1	B	399	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	501	LEU	CB-CG-CD1	-5.47	101.71	111.00
2	D	48	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	557	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	404	THR	N-CA-CB	5.26	120.29	110.30
2	D	97	GLU	CA-CB-CG	-5.23	101.89	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	503	ALA	CB-CA-C	-5.21	102.29	110.10
2	E	27	ASP	CB-CG-OD1	5.16	122.94	118.30
2	D	19	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	437	LEU	CB-CG-CD2	-5.07	102.39	111.00
2	D	78	THR	CA-CB-CG2	-5.03	105.36	112.40
1	B	530	VAL	CG1-CB-CG2	-5.01	102.88	110.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472[B]	LEU	Peptide
1	A	474[B]	ASN	Peptide
1	A	507[B]	SER	Peptide
1	B	469[B]	ASN	Peptide
1	C	397	ASP	Peptide
1	C	490	THR	Peptide

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	1499	0	1467	35	0
1	B	1402	0	1373	29	0
1	C	1374	0	1348	19	0
2	D	1172	0	1166	40	0
2	E	1167	0	1154	17	0
2	F	1143	0	1130	30	0
3	A	201	0	0	10	1
3	B	178	0	0	13	1
3	C	132	0	0	6	0
3	D	102	0	0	8	1
3	E	74	0	0	1	1
3	F	48	0	0	7	0
All	All	8492	0	7638	165	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:GLN:HG3	3:D:2091:HOH:O	1.40	1.19
1:B:481:ARG:C	3:B:2079:HOH:O	1.84	1.13
2:D:126[B]:LEU:HD13	2:D:164:ILE:CD1	1.80	1.12
1:A:473[B]:ASN:HB3	3:A:2082:HOH:O	1.49	1.09
1:A:474[B]:ASN:OD1	1:A:475[B]:SER:O	1.71	1.08
1:B:581:GLU:CD	3:B:2178:HOH:O	1.95	1.03
1:A:519:GLN:HG2	3:A:2119:HOH:O	1.58	1.02
1:B:581:GLU:OE1	3:B:2178:HOH:O	1.84	0.94
3:B:2041:HOH:O	2:E:78:THR:HG23	1.67	0.93
2:F:31:ARG:HH12	2:F:68:ARG:HH22	1.15	0.93
1:B:481:ARG:NH2	3:B:2081:HOH:O	1.92	0.91
2:D:31:ARG:HB2	2:D:31:ARG:HH11	1.36	0.91
1:B:519[B]:GLN:NE2	3:B:2115:HOH:O	2.06	0.89
2:D:126[B]:LEU:CD1	2:D:164:ILE:CD1	2.51	0.88
2:D:61:GLU:HB3	3:D:2020:HOH:O	1.74	0.88
2:D:31:ARG:NH1	2:D:31:ARG:HB2	1.89	0.86
1:B:399:LEU:N	3:B:2001:HOH:O	2.08	0.85
1:A:506[B]:LYS:O	1:A:507[B]:SER:CB	2.25	0.84
1:A:506[B]:LYS:O	1:A:507[B]:SER:HB2	1.76	0.84
2:E:34:MET:HA	2:E:34:MET:HE2	1.62	0.82
2:F:34:MET:HE2	2:F:34:MET:HA	1.61	0.81
1:A:511:THR:HG21	3:A:2099:HOH:O	1.81	0.80
2:D:126[B]:LEU:CD1	2:D:164:ILE:HD13	2.12	0.79
2:D:68:ARG:NH2	3:D:2022:HOH:O	2.16	0.78
1:C:398:LYS:H	1:C:398:LYS:HD3	1.50	0.77
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD13	1.67	0.75
1:C:519:GLN:HG2	3:C:2084:HOH:O	1.87	0.75
1:A:474[B]:ASN:CG	1:A:475[B]:SER:O	2.25	0.75
1:B:506[A]:LYS:HE2	1:B:548:SER:O	1.88	0.74
1:B:519[B]:GLN:CD	3:B:2115:HOH:O	2.26	0.74
2:F:135:HIS:HD2	3:F:2027:HOH:O	1.70	0.74
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD11	1.68	0.73
1:A:507[B]:SER:OG	1:A:540:GLN:HB2	1.88	0.73
1:C:508:HIS:HD2	3:C:2075:HOH:O	1.71	0.73
2:D:126[B]:LEU:HD12	2:D:126[B]:LEU:O	1.89	0.72
1:A:505:PRO:O	1:A:508[B]:HIS:HB2	1.89	0.72
2:F:29:GLU:O	2:F:33:LEU:HD23	1.89	0.72
1:A:473[A]:ASN:OD1	3:A:2081:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ASN:C	1:C:490:THR:HG23	2.10	0.72
2:D:23:ARG:O	2:D:23:ARG:HG2	1.89	0.71
1:B:519[A]:GLN:NE2	3:B:2112:HOH:O	2.15	0.71
2:F:31:ARG:NH1	2:F:68:ARG:HH22	1.88	0.70
2:F:144:LYS:HG3	2:F:145:PHE:H	1.55	0.70
2:F:18:LEU:HD22	2:F:34:MET:HE1	1.72	0.69
1:A:471:LEU:HD22	1:A:475[B]:SER:HB2	1.76	0.68
2:F:142:GLN:HG2	2:F:148:THR:HG22	1.76	0.66
2:F:91:GLY:O	3:F:2021:HOH:O	2.14	0.66
1:A:475[B]:SER:C	1:A:477:LEU:N	2.49	0.65
3:B:2043:HOH:O	2:E:78:THR:HG21	1.97	0.65
1:B:468:LEU:O	1:B:469[B]:ASN:HB3	1.97	0.64
1:B:470[A]:ASN:HA	1:B:475:PRO:HD3	1.77	0.64
1:A:511:THR:CG2	3:A:2099:HOH:O	2.41	0.64
1:A:493:ASN:ND2	3:A:2074:HOH:O	2.31	0.63
2:E:25:GLY:HA3	2:E:59:HIS:CE1	2.34	0.63
2:D:126[B]:LEU:CD1	2:D:164:ILE:HD11	2.26	0.63
2:D:144:LYS:CB	2:D:144:LYS:NZ	2.61	0.62
2:E:82:THR:H	2:E:85:HIS:HD2	1.47	0.62
2:F:59:HIS:CD2	3:F:2011:HOH:O	2.51	0.62
2:E:165:LEU:O	2:E:166:GLN:NE2	2.33	0.62
2:F:59:HIS:HD2	3:F:2011:HOH:O	1.82	0.61
1:A:474[A]:ASN:HA	1:A:479:PRO:HD3	1.81	0.61
1:A:473[B]:ASN:CB	3:A:2082:HOH:O	2.23	0.59
1:B:468:LEU:O	1:B:469[A]:ASN:HB3	2.03	0.59
2:D:135:HIS:HE1	3:D:2041:HOH:O	1.85	0.59
1:B:470[A]:ASN:HD22	1:B:470[A]:ASN:C	2.06	0.58
2:E:82:THR:H	2:E:85:HIS:CD2	2.21	0.58
2:D:126[B]:LEU:HD12	2:D:126[B]:LEU:C	2.25	0.57
2:F:18:LEU:HD22	2:F:34:MET:CE	2.35	0.57
2:F:53:MET:O	2:F:57:VAL:HG23	2.04	0.57
1:C:398:LYS:N	1:C:398:LYS:HD3	2.19	0.56
2:D:29:GLU:HG3	2:D:33:LEU:HD22	1.87	0.56
1:A:507[B]:SER:C	1:A:509[B]:GLY:H	2.08	0.56
2:D:118:TYR:OH	2:D:152:ILE:HD11	2.04	0.56
2:F:92:HIS:HD2	3:F:2023:HOH:O	1.89	0.56
1:C:469:ASN:HA	3:C:2056:HOH:O	2.05	0.56
1:A:473[A]:ASN:CG	1:A:474[A]:ASN:H	2.10	0.55
2:D:25:GLY:HA3	2:D:59:HIS:CE1	2.42	0.54
1:C:468:LEU:O	1:C:471:SER:HB2	2.07	0.54
2:D:166:GLN:C	3:D:2088:HOH:O	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:ASN:HB2	1:C:490:THR:CG2	2.38	0.53
1:B:458:ILE:HG12	1:B:553[A]:SER:HB2	1.89	0.53
2:E:85:HIS:HE1	2:E:114:ILE:O	1.92	0.53
2:D:118:TYR:CZ	2:D:152:ILE:HD12	2.44	0.52
1:C:469:ASN:O	1:C:470:ASN:HB2	2.09	0.52
2:F:85:HIS:HE1	2:F:114:ILE:O	1.93	0.52
1:B:506[A]:LYS:O	1:B:507[A]:SER:HB2	2.09	0.52
2:F:29:GLU:HG3	2:F:33:LEU:HD21	1.92	0.52
1:C:403:THR:HA	1:C:477:TYR:O	2.08	0.52
1:A:473[A]:ASN:CG	1:A:474[A]:ASN:N	2.63	0.52
2:E:165:LEU:O	2:E:166:GLN:CD	2.48	0.52
1:B:468:LEU:O	1:B:469[B]:ASN:CB	2.58	0.51
1:A:526[B]:LYS:CE	3:A:2127:HOH:O	2.58	0.51
2:D:118:TYR:CZ	2:D:152:ILE:CD1	2.94	0.51
2:E:18:LEU:HD22	2:E:34:MET:HE1	1.93	0.51
1:C:463:GLU:H	1:C:463:GLU:CD	2.15	0.51
2:D:32:ILE:O	2:D:35:ALA:HB3	2.11	0.50
2:F:82:THR:H	2:F:85:HIS:CD2	2.30	0.50
2:E:32:ILE:O	2:E:35:ALA:HB3	2.11	0.50
1:B:526:LYS:HE3	1:C:557:ASP:CG	2.31	0.50
1:A:506[B]:LYS:O	1:A:507[B]:SER:OG	2.30	0.50
2:F:144:LYS:HG3	2:F:145:PHE:N	2.27	0.49
2:D:144:LYS:NZ	2:D:144:LYS:HB3	2.26	0.49
2:F:27:ASP:OD1	2:F:62:ILE:HG13	2.12	0.49
2:F:34:MET:CA	2:F:34:MET:HE2	2.36	0.49
2:D:144:LYS:HB3	2:D:144:LYS:HZ3	1.77	0.49
1:A:473[A]:ASN:OD1	1:A:475[A]:SER:HB2	2.12	0.49
2:F:29:GLU:HG3	2:F:33:LEU:CD2	2.43	0.48
2:F:15:GLY:N	3:F:2001:HOH:O	2.46	0.48
1:B:523:ASN:HA	1:C:512:ALA:HB2	1.95	0.48
2:D:125:HIS:HD2	3:D:2098:HOH:O	1.95	0.48
2:D:126[B]:LEU:HD13	2:D:164:ILE:HD12	1.86	0.48
1:A:473[A]:ASN:ND2	1:A:474[A]:ASN:H	2.12	0.48
2:E:34:MET:CE	2:E:34:MET:HA	2.41	0.47
2:F:142:GLN:HA	2:F:147:LYS:O	2.15	0.47
2:F:82:THR:H	2:F:85:HIS:HD2	1.61	0.47
2:F:145:PHE:HB2	2:F:147:LYS:HE2	1.96	0.47
2:D:144:LYS:NZ	2:D:144:LYS:HB2	2.29	0.47
2:E:18:LEU:HA	2:E:33:LEU:HD23	1.98	0.46
1:B:403:THR:HA	1:B:477:TYR:O	2.16	0.46
2:D:118:TYR:CE2	2:D:152:ILE:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:CYS:HA	1:A:476[B]:PHE:O	2.15	0.46
2:D:159:GLU:O	2:D:163:GLU:HG3	2.16	0.45
3:B:2041:HOH:O	2:E:78:THR:CG2	2.43	0.45
1:B:445:LEU:HB2	3:B:2040:HOH:O	2.15	0.45
1:C:456:HIS:HE1	3:C:2099:HOH:O	1.98	0.45
1:C:541:GLU:HG2	1:C:546:THR:O	2.17	0.45
1:C:482:ASN:HB2	1:C:490:THR:HG21	1.98	0.45
2:D:153:SER:OG	2:D:161:LEU:CD2	2.64	0.45
2:D:153:SER:OG	2:D:161:LEU:HD23	2.17	0.45
1:B:469[B]:ASN:C	1:B:471[B]:SER:N	2.70	0.45
2:D:29:GLU:N	3:D:2004:HOH:O	2.41	0.45
1:B:505:PRO:O	1:B:508[A]:HIS:HB2	2.17	0.45
2:E:125:HIS:HD2	3:E:2055:HOH:O	2.00	0.44
1:A:507[B]:SER:C	1:A:509[B]:GLY:N	2.70	0.44
1:A:517:VAL:HB	1:C:521:TYR:CD2	2.53	0.44
2:F:100:LEU:HD13	2:F:135:HIS:CG	2.53	0.44
1:C:526:LYS:HE2	3:C:2089:HOH:O	2.18	0.44
2:D:26:GLN:O	2:D:27:ASP:C	2.54	0.43
2:F:94:GLU:HG3	3:F:2025:HOH:O	2.18	0.43
2:F:144:LYS:CG	2:F:145:PHE:H	2.28	0.43
1:B:469[B]:ASN:C	1:B:471[B]:SER:H	2.21	0.43
2:E:160:ASP:O	2:E:164:ILE:HG13	2.19	0.43
1:A:407:THR:HA	1:A:481:TYR:O	2.19	0.43
1:B:402:TRP:CZ2	1:B:481:ARG:HG3	2.54	0.43
1:A:430:THR:HG21	1:B:428:CYS:O	2.19	0.43
1:C:469:ASN:C	1:C:471:SER:H	2.21	0.42
2:D:166:GLN:CG	3:D:2091:HOH:O	2.22	0.42
1:B:509[A]:GLY:N	3:B:2100:HOH:O	2.37	0.42
2:E:150[A]:PHE:CE1	2:E:165:LEU:HB3	2.55	0.42
1:A:485:ARG:NH1	3:A:2087:HOH:O	2.52	0.42
1:A:521:TYR:CD1	1:B:517:VAL:HB	2.54	0.42
1:A:476[B]:PHE:N	1:A:476[B]:PHE:CD1	2.86	0.42
1:A:476[B]:PHE:N	1:A:476[B]:PHE:HD1	2.18	0.41
2:D:144:LYS:HZ2	2:D:144:LYS:HB2	1.85	0.41
1:A:526[B]:LYS:NZ	3:A:2127:HOH:O	2.49	0.41
1:A:506[B]:LYS:HE3	1:A:539:THR:O	2.21	0.41
1:B:470[A]:ASN:ND2	1:B:470[A]:ASN:C	2.71	0.41
2:D:126[A]:LEU:HD22	2:D:161:LEU:HD13	2.03	0.41
2:D:34:MET:HE2	2:D:40:ALA:HB2	2.04	0.40
1:B:526:LYS:HD2	3:C:2096:HOH:O	2.20	0.40
2:F:155:ASP:C	2:F:157:GLY:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:VAL:O	2:F:34:MET:HG2	2.21	0.40

All (2) 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)
3:B:2170:HOH:O	3:E:2038:HOH:O[3_555]	2.14	0.06
3:A:2183:HOH:O	3:D:2078: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	194/201 (96%)	175 (90%)	9 (5%)	10 (5%)	2 0
1	B	178/201 (89%)	164 (92%)	8 (4%)	6 (3%)	5 0
1	C	173/201 (86%)	162 (94%)	11 (6%)	0	100 100
2	D	154/154 (100%)	151 (98%)	1 (1%)	2 (1%)	15 4
2	E	153/154 (99%)	152 (99%)	1 (1%)	0	100 100
2	F	150/154 (97%)	138 (92%)	9 (6%)	3 (2%)	9 2
All	All	1002/1065 (94%)	942 (94%)	39 (4%)	21 (2%)	15 2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	474[A]	ASN
1	A	474[B]	ASN
1	A	476[A]	PHE
1	A	476[B]	PHE
1	A	507[A]	SER
1	A	507[B]	SER

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Mol	Chain	Res	Type
1	A	508[A]	HIS
1	A	508[B]	HIS
1	B	470[A]	ASN
1	B	470[B]	ASN
1	B	472[A]	PHE
1	B	472[B]	PHE
1	A	473[A]	ASN
1	A	473[B]	ASN
2	D	155	ASP
2	D	156	ILE
2	F	144	LYS
2	F	155	ASP
1	B	469[A]	ASN
1	B	469[B]	ASN
2	F	156	ILE

5.3.2 Protein sidechains

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	169/171 (99%)	162 (96%)	7 (4%)	37 22
1	B	158/171 (92%)	151 (96%)	7 (4%)	35 19
1	C	156/171 (91%)	147 (94%)	9 (6%)	25 10
2	D	119/117 (102%)	115 (97%)	4 (3%)	44 30
2	E	118/117 (101%)	109 (92%)	9 (8%)	16 5
2	F	115/117 (98%)	107 (93%)	8 (7%)	19 6
All	All	835/864 (97%)	791 (95%)	44 (5%)	29 13

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	402	LYS
1	A	406	TRP

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Mol	Chain	Res	Type
1	A	488	ASP
1	A	489	LEU
1	A	493	ASN
1	A	562	ASN
1	B	402	TRP
1	B	469[A]	ASN
1	B	469[B]	ASN
1	B	470[A]	ASN
1	B	470[B]	ASN
1	B	479	ASN
1	B	562	ASN
1	C	397	ASP
1	C	398	LYS
1	C	402	TRP
1	C	469	ASN
1	C	490	THR
1	C	491	GLU
1	C	508	HIS
1	C	545	THR
1	C	562	ASN
2	D	14	LEU
2	D	31	ARG
2	D	33	LEU
2	D	144	LYS
2	E	28	ASP
2	E	31	ARG
2	E	33	LEU
2	E	61	GLU
2	E	106	VAL
2	E	139	VAL
2	E	147	LYS
2	E	163	GLU
2	E	166	GLN
2	F	16	LYS
2	F	28	ASP
2	F	33	LEU
2	F	139	VAL
2	F	147	LYS
2	F	152	ILE
2	F	154	ILE
2	F	159	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	A	486	ASN
1	A	493	ASN
1	A	562	ASN
1	B	431	GLN
1	B	562	ASN
1	C	431	GLN
1	C	470	ASN
1	C	493	ASN
1	C	562	ASN
2	D	26	GLN
2	D	59	HIS
2	D	85	HIS
2	D	125	HIS
2	E	26	GLN
2	E	59	HIS
2	E	85	HIS
2	E	125	HIS
2	E	166	GLN
2	F	59	HIS
2	F	85	HIS
2	F	125	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	182/201 (90%)	0.74	23 (12%)	5 8	21, 28, 57, 94	0
1	B	171/201 (85%)	0.92	28 (16%)	2 3	21, 30, 60, 75	0
1	C	176/201 (87%)	0.90	30 (17%)	2 3	22, 35, 89, 116	0
2	D	154/154 (100%)	0.48	16 (10%)	8 13	26, 39, 76, 99	0
2	E	154/154 (100%)	0.65	24 (15%)	3 4	28, 46, 82, 104	0
2	F	152/154 (98%)	2.36	68 (44%)	0 0	37, 59, 110, 122	0
All	All	989/1065 (92%)	0.99	189 (19%)	2 2	21, 37, 89, 122	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	161	LEU	10.6
2	F	145	PHE	10.5
2	F	165	LEU	9.9
2	F	164	ILE	9.0
2	F	154	ILE	8.4
2	F	156	ILE	8.1
2	F	32	ILE	7.8
1	C	542	THR	7.7
2	F	162	ALA	7.6
2	F	166	GLN	7.6
1	C	470	ASN	7.1
2	F	150	PHE	7.0
2	F	35	ALA	6.8
2	F	163	GLU	6.8
2	F	159	GLU	6.6
1	C	545	THR	6.3
2	F	157	GLY	6.3
1	A	490	THR	6.1
2	F	31	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	546	THR	5.8
2	D	35	ALA	5.8
1	B	509[A]	GLY	5.8
2	F	152	ILE	5.7
1	A	509[A]	GLY	5.7
2	F	30	VAL	5.5
2	F	37	GLY	5.4
2	F	34	MET	5.2
1	C	547	PRO	5.2
2	F	158	ASN	4.9
2	F	33	LEU	4.9
2	F	133	LEU	4.9
1	B	544	ASP	4.8
2	E	32	ILE	4.8
1	C	469	ASN	4.8
2	F	144	LYS	4.8
2	F	146	GLY	4.6
1	B	543	GLY	4.6
1	C	541	GLU	4.4
2	F	160	ASP	4.4
2	F	155	ASP	4.3
2	F	68	ARG	4.3
1	C	477	TYR	4.3
2	F	139	VAL	4.2
1	C	492	GLY	4.2
1	B	470[A]	ASN	4.2
2	E	14	LEU	4.2
2	F	142	GLN	4.1
2	F	36	ASN	4.1
1	C	540	GLN	4.1
1	A	489	LEU	4.0
2	D	32	ILE	3.9
2	F	27	ASP	3.8
2	F	93	LEU	3.8
2	D	36	ASN	3.8
2	F	38	ALA	3.7
1	B	508[A]	HIS	3.7
2	E	13	ASP	3.7
2	E	28	ASP	3.7
2	F	126	LEU	3.6
2	F	129	VAL	3.6
2	D	14	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	542	THR	3.5
1	B	433	LEU	3.5
2	F	153	SER	3.4
2	D	28	ASP	3.4
2	E	36	ASN	3.4
2	F	134	LYS	3.4
1	B	471[A]	SER	3.4
2	E	31	ARG	3.3
1	C	482	ASN	3.3
2	E	163	GLU	3.3
2	F	130	GLU	3.3
2	E	162	ALA	3.3
1	C	491	GLU	3.2
2	E	35	ALA	3.2
1	B	575	PHE	3.2
2	E	37	GLY	3.2
1	A	437	LEU	3.2
2	F	140	ASN	3.2
1	C	415	ALA	3.1
2	F	118	TYR	3.1
1	B	573	TYR	3.1
1	C	434	ALA	3.1
1	C	433	LEU	3.1
2	F	29	GLU	3.1
1	B	516	ILE	3.1
2	F	67	LEU	3.1
2	F	148	THR	3.1
1	B	434	ALA	3.0
1	A	508[A]	HIS	3.0
2	D	34	MET	3.0
1	A	473[A]	ASN	3.0
2	F	64	GLU	3.0
2	E	145	PHE	2.9
1	A	488	ASP	2.9
2	F	65	VAL	2.9
2	E	33	LEU	2.9
2	F	18	LEU	2.9
2	D	159	GLU	2.9
2	E	150[A]	PHE	2.9
1	B	469[A]	ASN	2.9
1	C	472	PHE	2.8
1	A	575	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	159	GLU	2.8
2	F	151	ASP	2.8
2	D	31	ARG	2.8
2	F	137	ALA	2.8
1	C	517	VAL	2.8
2	E	161	LEU	2.7
2	F	143	ASP	2.7
2	E	34	MET	2.7
2	D	30	VAL	2.7
1	C	574	THR	2.7
2	F	117	LEU	2.7
2	E	164	ILE	2.6
2	F	95	ILE	2.6
1	C	575	PHE	2.6
1	B	436	VAL	2.6
1	A	573	TYR	2.6
1	C	490	THR	2.6
1	A	491	GLU	2.6
2	F	28	ASP	2.6
1	C	507	SER	2.6
2	D	166	GLN	2.6
1	A	438	ALA	2.6
2	E	166	GLN	2.5
2	D	13	ASP	2.5
1	C	476	GLU	2.5
1	B	520	VAL	2.5
2	F	63	VAL	2.5
2	F	16	LYS	2.5
1	C	516	ILE	2.5
1	B	424	VAL	2.5
1	B	432	ILE	2.5
1	B	507[A]	SER	2.5
1	A	440	VAL	2.4
2	F	94	GLU	2.4
1	A	475[A]	SER	2.4
2	E	158	ASN	2.4
2	F	26	GLN	2.4
2	F	97	GLU	2.4
1	B	517	VAL	2.4
1	A	507[A]	SER	2.4
1	B	521	TYR	2.3
2	F	121	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	156	ILE	2.3
1	C	428	CYS	2.3
1	B	532	LEU	2.3
1	B	574	THR	2.3
2	D	160	ASP	2.3
1	A	474[A]	ASN	2.3
1	B	435	THR	2.3
1	C	416	GLU	2.3
2	E	61	GLU	2.3
1	B	425	LEU	2.3
2	D	29	GLU	2.3
1	A	516	ILE	2.3
1	C	432	ILE	2.3
2	F	70	GLY	2.3
1	B	536	LEU	2.2
2	D	33	LEU	2.2
1	A	520	VAL	2.2
1	A	534	ILE	2.2
2	F	43	TYR	2.2
1	A	532	LEU	2.2
2	D	37	GLY	2.2
2	F	112	THR	2.2
1	C	534	ILE	2.2
1	A	521	TYR	2.2
1	A	439	THR	2.2
2	E	27	ASP	2.2
1	B	571	SER	2.2
1	A	574	THR	2.1
2	E	30	VAL	2.1
2	F	25	GLY	2.1
1	C	518[A]	SER	2.1
2	E	154	ILE	2.1
1	B	423	LEU	2.1
2	F	40	ALA	2.1
1	C	471	SER	2.1
2	F	39	ASP	2.1
1	C	578	ILE	2.0
2	F	42	ALA	2.0
2	F	100	LEU	2.0
1	B	546	THR	2.0
2	F	147	LYS	2.0
1	A	436	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	60	LEU	2.0
2	D	27	ASP	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.