Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:15 AM GMT

PDB ID	:	2CE9
Title	:	A WRPW PEPTIDE BOUND TO THE GROUCHO-TLE WD40 DOMAIN.
Authors	:	Pickles, L.M.; Roe, S.M.; Pearl, L.H.
Deposited on	:	2006-02-03
Resolution	:	2.12 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:

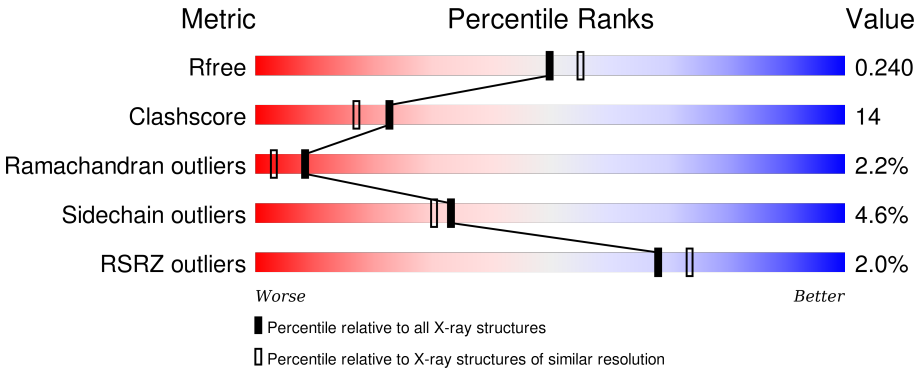
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.12 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	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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	337	% 78% 18% ·
1	B	337	3% 79% 18% ··
1	C	337	% 82% 14% ·
1	D	337	3% 74% 18% 5% ··
2	X	5	80% 20%

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Mol	Chain	Length	Quality of chain
2	Y	5	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11285 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 TRANSDUCIN-LIKE ENHANCER PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	B	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	C	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	D	332	Total	C	N	O	S	0	0	0
			2554	1610	439	488	17			

- Molecule 2 is a protein called WRPW PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	S	0	0	0
			55	38	10	6	1			
2	Y	5	Total	C	N	O	S	0	0	0
			54	38	10	5	1			

- Molecule 3 is water.

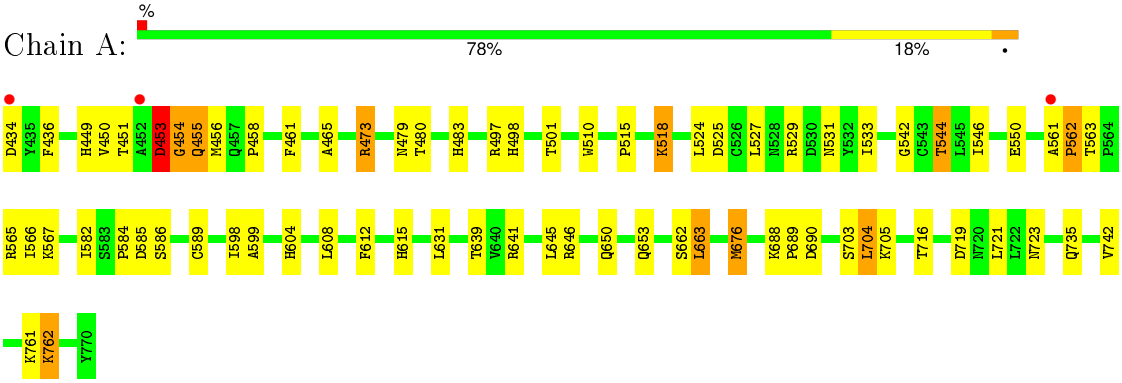
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	228	Total	O	0	0
			228	228		
3	C	206	Total	O	0	0
			206	206		
3	D	176	Total	O	0	0
			176	176		
3	X	3	Total	O	0	0
			3	3		
3	Y	2	Total	O	0	0
			2	2		

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.

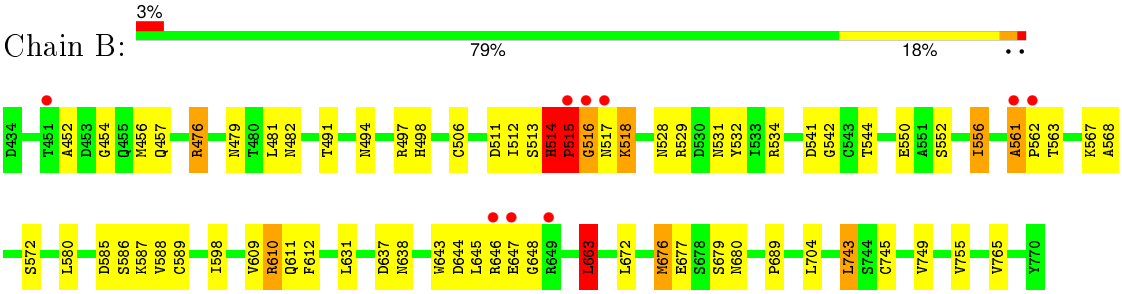
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain A:



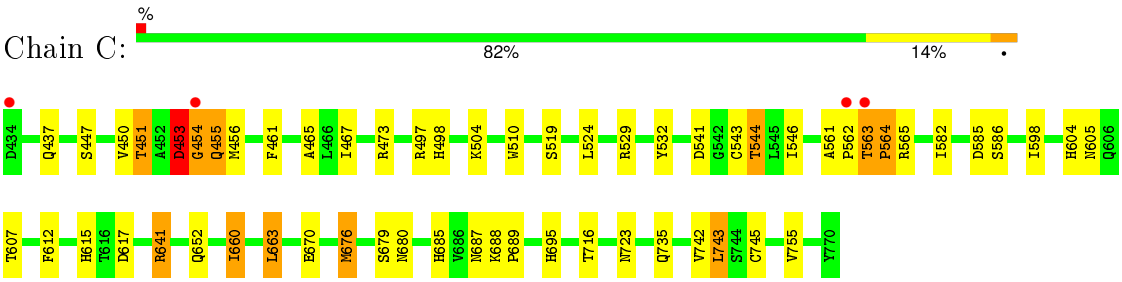
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain B:



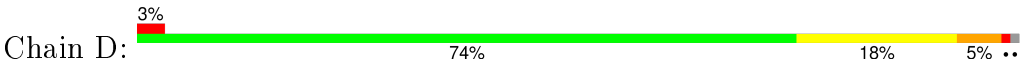
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

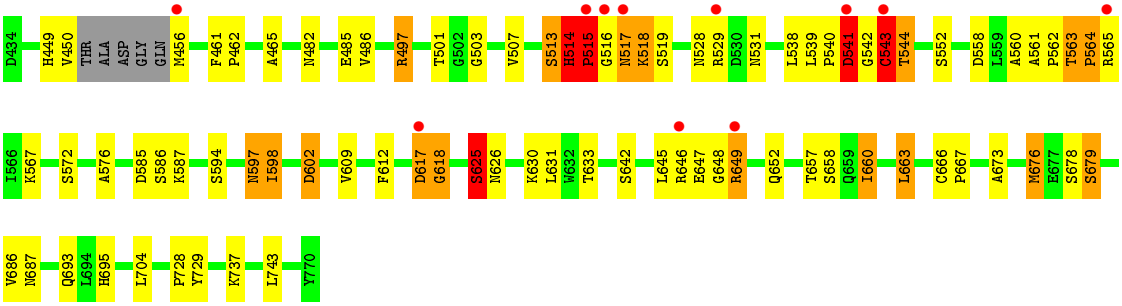
Chain C:



• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain D:





- Molecule 2: WRPW PEPTIDE

Chain X:

- Molecule 2: WRPW PEPTIDE

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.81Å 56.48Å 126.64Å 90.00° 112.68° 90.00°	Depositor
Resolution (Å)	117.04 – 2.12 42.48 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.7 (117.04-2.12) 97.6 (42.48-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.244 0.177 , 0.240	Depositor DCC
R_{free} test set	3924 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.8	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	3 of 77993 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11285	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 83.94 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9016e-07.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.98	3/2653 (0.1%)	0.98	10/3612 (0.3%)
1	B	0.94	1/2653 (0.0%)	1.00	8/3612 (0.2%)
1	C	0.90	0/2653	0.89	6/3612 (0.2%)
1	D	0.87	1/2619 (0.0%)	0.95	11/3564 (0.3%)
2	X	0.87	0/59	0.68	0/79
2	Y	0.82	0/58	0.83	0/79
All	All	0.92	5/10695 (0.0%)	0.95	35/14558 (0.2%)

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	2
1	B	0	2
1	C	0	1
1	D	0	4
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	CYS	CB-SG	-6.45	1.71	1.82
1	A	762	LYS	CD-CE	6.00	1.66	1.51
1	A	762	LYS	CE-NZ	5.74	1.63	1.49
1	A	589	CYS	CB-SG	-5.20	1.73	1.81
1	D	485	GLU	CG-CD	5.03	1.59	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	514	HIS	C-N-CD	-18.97	78.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	514	HIS	C-N-CA	13.80	179.96	122.00
1	A	704	LEU	CA-CB-CG	11.45	141.63	115.30
1	D	514	HIS	C-N-CD	-11.14	96.08	120.60
1	A	473	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	473	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	C	641	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	704	LEU	CA-CB-CG	8.82	135.58	115.30
1	A	676	MET	CG-SD-CE	-8.10	87.24	100.20
1	B	704	LEU	CB-CG-CD2	-8.00	97.40	111.00
1	C	641	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	D	514	HIS	C-N-CA	7.58	153.82	122.00
1	B	515	PRO	CA-N-CD	-7.43	101.09	111.50
1	A	704	LEU	CB-CG-CD1	-7.09	98.95	111.00
1	C	454	GLY	N-CA-C	6.64	129.71	113.10
1	D	704	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	D	515	PRO	N-CA-C	6.42	128.80	112.10
1	B	704	LEU	CB-CG-CD1	-6.37	100.17	111.00
1	A	663	LEU	CA-CB-CG	6.33	129.85	115.30
1	D	515	PRO	CA-N-CD	-6.17	102.86	111.50
1	B	663	LEU	CA-CB-CG	5.67	128.35	115.30
1	D	538	LEU	CB-CG-CD2	-5.66	101.37	111.00
1	A	525	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	602	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	743	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	538	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	719	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	617	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	473	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	598	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	A	566	ILE	CG1-CB-CG2	-5.20	99.97	111.40
1	A	721	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	743	LEU	CA-CB-CG	5.13	127.10	115.30
1	D	663	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	704	LEU	CB-CG-CD2	-5.07	102.39	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	ASP	Peptide
1	A	454	GLY	Peptide
1	B	514	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	561	ALA	Peptide
1	C	453	ASP	Peptide
1	D	513	SER	Peptide
1	D	514	HIS	Peptide
1	D	515	PRO	Peptide
1	D	541	ASP	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	2587	0	2503	62	0
1	B	2587	0	2503	72	0
1	C	2587	0	2503	52	0
1	D	2554	0	2475	92	0
2	X	55	0	48	4	0
2	Y	54	0	48	1	0
3	A	246	0	0	29	0
3	B	228	0	0	16	0
3	C	206	0	0	12	0
3	D	176	0	0	13	0
3	X	3	0	0	0	0
3	Y	2	0	0	0	0
All	All	11285	0	10080	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (279) 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:D:517:ASN:HA	1:D:518:LYS:CB	1.46	1.38
1:D:517:ASN:CA	1:D:518:LYS:HB2	1.63	1.27
1:C:563:THR:HB	1:C:564:PRO:CD	1.64	1.24
1:C:454:GLY:HA2	1:C:455:GLN:CB	1.66	1.23
1:A:762:LYS:HD2	3:A:2219:HOH:O	1.36	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:GLY:CA	1:D:543:CYS:HB3	1.70	1.21
1:D:514:HIS:CD2	1:D:515:PRO:HB2	1.77	1.19
1:D:543:CYS:SG	1:D:544:THR:HG22	1.81	1.18
1:A:762:LYS:HE3	3:A:2236:HOH:O	1.04	1.18
1:D:515:PRO:HG3	1:D:517:ASN:OD1	1.40	1.17
1:C:454:GLY:HA2	1:C:455:GLN:HB3	1.18	1.14
1:C:563:THR:CB	1:C:564:PRO:HD2	1.77	1.13
1:B:514:HIS:N	1:B:515:PRO:HD3	1.46	1.10
1:D:514:HIS:HD2	1:D:515:PRO:HB2	0.92	1.07
1:C:454:GLY:CA	1:C:455:GLN:HB3	1.85	1.06
1:D:542:GLY:HA2	1:D:543:CYS:HB3	1.32	1.04
1:B:749:VAL:HG22	3:B:2051:HOH:O	1.60	1.00
1:D:543:CYS:SG	1:D:544:THR:CG2	2.50	0.99
1:B:517:ASN:HA	1:B:518:LYS:HB3	1.44	0.99
1:D:541:ASP:HB2	1:D:543:CYS:SG	2.04	0.98
1:B:513:SER:C	1:B:515:PRO:HD3	1.87	0.93
1:C:565:ARG:HG3	3:C:2076:HOH:O	1.68	0.91
1:D:517:ASN:HA	1:D:518:LYS:HB3	1.51	0.91
1:C:563:THR:HB	1:C:564:PRO:HD2	0.92	0.91
1:A:705:LYS:HE3	3:A:2198:HOH:O	1.71	0.89
1:D:517:ASN:HA	1:D:518:LYS:HB2	0.91	0.89
1:D:542:GLY:N	1:D:543:CYS:HB3	1.85	0.89
1:B:515:PRO:C	1:B:517:ASN:H	1.74	0.88
1:D:517:ASN:CA	1:D:518:LYS:CB	2.34	0.87
1:B:515:PRO:HG2	1:B:516:GLY:H	1.40	0.86
1:D:676:MET:HA	1:D:676:MET:CE	2.07	0.84
1:C:561:ALA:O	1:C:563:THR:HA	1.78	0.84
1:B:515:PRO:CG	1:B:516:GLY:H	1.92	0.83
1:C:544:THR:HG23	3:C:2067:HOH:O	1.77	0.83
1:D:515:PRO:CG	1:D:517:ASN:OD1	2.27	0.82
1:C:456:MET:HE1	3:C:2148:HOH:O	1.80	0.81
1:C:561:ALA:HB1	3:C:2075:HOH:O	1.80	0.81
1:B:514:HIS:N	1:B:515:PRO:CD	2.39	0.80
1:B:517:ASN:HA	1:B:518:LYS:CB	2.02	0.79
1:D:515:PRO:HG3	1:D:517:ASN:CG	2.02	0.79
1:D:515:PRO:HB3	1:D:517:ASN:HB2	1.64	0.78
1:A:515:PRO:HA	3:A:2058:HOH:O	1.84	0.78
1:A:454:GLY:HA2	1:A:455:GLN:HB2	1.64	0.78
1:A:639:THR:OG1	1:A:641:ARG:NH1	2.16	0.78
1:C:454:GLY:HA2	1:C:455:GLN:HB2	1.61	0.77
1:D:676:MET:HE3	1:D:676:MET:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:VAL:HG22	1:D:456:MET:HG2	1.64	0.76
1:A:544:THR:HG23	3:A:2083:HOH:O	1.84	0.76
1:D:514:HIS:HD2	1:D:515:PRO:CB	1.86	0.76
1:A:688:LYS:HB3	1:A:689:PRO:HD2	1.66	0.75
1:D:486:VAL:CG1	1:D:743:LEU:HD21	2.17	0.75
1:D:585:ASP:OD1	1:D:587:LYS:HG2	1.87	0.74
1:D:649:ARG:HG2	3:D:2103:HOH:O	1.87	0.74
1:C:563:THR:CB	1:C:564:PRO:CD	2.52	0.73
1:B:646:ARG:HG2	3:B:2138:HOH:O	1.87	0.73
1:B:514:HIS:ND1	1:B:515:PRO:HG3	2.04	0.72
1:C:450:VAL:HG22	1:C:456:MET:HG2	1.71	0.71
1:D:695:HIS:HE1	3:D:2131:HOH:O	1.72	0.71
1:D:542:GLY:HA2	1:D:543:CYS:CB	2.19	0.70
1:C:723:ASN:HD21	1:C:735:GLN:HE21	1.39	0.70
1:A:434:ASP:HB2	3:A:2002:HOH:O	1.90	0.70
1:B:516:GLY:O	1:B:518:LYS:HA	1.92	0.69
1:B:528:ASN:HD22	1:B:531:ASN:CG	1.96	0.69
1:D:539:LEU:HD12	1:D:544:THR:HG23	1.75	0.68
1:D:517:ASN:N	1:D:518:LYS:HB2	2.07	0.68
1:C:543:CYS:SG	3:C:2066:HOH:O	2.51	0.68
1:B:631:LEU:HB2	1:B:645:LEU:HD21	1.75	0.68
1:D:528:ASN:HB3	1:D:531:ASN:ND2	2.09	0.68
1:B:515:PRO:C	1:B:517:ASN:N	2.43	0.67
1:B:585:ASP:OD1	1:B:587:LYS:HG2	1.93	0.67
1:B:529:ARG:NH2	3:B:2070:HOH:O	2.26	0.67
1:A:436:PHE:O	1:A:473:ARG:NH2	2.27	0.67
1:A:567:LYS:HE3	3:A:2097:HOH:O	1.93	0.67
1:D:482:ASN:ND2	3:D:2025:HOH:O	2.28	0.66
1:D:552:SER:HB2	3:D:2059:HOH:O	1.94	0.66
1:C:723:ASN:HD22	1:C:735:GLN:HG2	1.59	0.66
1:B:482:ASN:ND2	3:B:2039:HOH:O	2.27	0.66
1:D:486:VAL:HG13	1:D:743:LEU:HD21	1.77	0.65
1:D:542:GLY:CA	1:D:543:CYS:CB	2.61	0.64
1:A:561:ALA:HB1	3:A:2093:HOH:O	1.98	0.64
1:A:498:HIS:HD2	3:A:2047:HOH:O	1.81	0.63
1:B:452:ALA:HB2	1:B:689:PRO:HG2	1.80	0.63
1:D:515:PRO:CB	1:D:517:ASN:HB2	2.28	0.63
1:C:695:HIS:HE1	3:C:2154:HOH:O	1.81	0.63
1:A:518:LYS:HE2	3:A:2040:HOH:O	1.97	0.63
1:A:584:PRO:HD2	3:A:2108:HOH:O	1.99	0.62
1:A:550:GLU:HG2	2:X:2:MET:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:MET:HE2	1:D:676:MET:HA	1.82	0.61
1:D:737:LYS:HE2	3:D:2145:HOH:O	2.01	0.61
1:B:498:HIS:HD2	3:B:2046:HOH:O	1.82	0.61
1:A:562:PRO:HB2	3:A:2092:HOH:O	2.01	0.61
1:A:483:HIS:HD2	1:A:501:THR:OG1	1.83	0.61
1:A:705:LYS:HE2	3:A:2197:HOH:O	2.00	0.60
1:D:515:PRO:HB3	1:D:517:ASN:H	1.65	0.60
1:C:688:LYS:HB3	1:C:689:PRO:HD2	1.82	0.60
1:A:450:VAL:HG22	1:A:456:MET:HG3	1.84	0.60
1:B:515:PRO:CG	1:B:516:GLY:N	2.58	0.60
1:A:542:GLY:HA2	3:A:2084:HOH:O	2.03	0.59
1:A:449:HIS:HE1	1:A:690:ASP:OD2	1.85	0.59
1:C:605:ASN:O	1:C:607:THR:HG23	2.03	0.59
1:B:612:PHE:HE1	1:B:648:GLY:HA2	1.68	0.58
1:B:494:ASN:OD1	1:B:749:VAL:HG21	2.03	0.58
1:B:556:ILE:HG23	1:B:568:ALA:HB3	1.86	0.58
1:A:453:ASP:HB2	1:A:454:GLY:HA2	1.86	0.58
1:C:670:GLU:HG3	3:C:2140:HOH:O	2.03	0.57
1:B:528:ASN:HB3	1:B:531:ASN:ND2	2.18	0.57
1:B:532:TYR:CE2	3:B:2074:HOH:O	2.52	0.57
1:D:541:ASP:C	1:D:543:CYS:HB3	2.24	0.57
1:A:453:ASP:HB2	1:A:455:GLN:HB2	1.85	0.57
1:C:652:GLN:NE2	1:C:687:ASN:OD1	2.38	0.57
1:A:544:THR:HG21	3:A:2098:HOH:O	2.03	0.56
1:A:479:ASN:HB3	3:A:2039:HOH:O	2.05	0.56
1:A:453:ASP:OD1	1:A:453:ASP:N	2.37	0.56
1:B:532:TYR:HE1	3:B:2072:HOH:O	1.87	0.56
1:D:515:PRO:HG3	1:D:517:ASN:CB	2.35	0.56
1:B:644:ASP:OD2	1:B:646:ARG:HG3	2.06	0.56
1:A:449:HIS:HD2	3:A:2120:HOH:O	1.89	0.56
1:A:454:GLY:HA2	1:A:455:GLN:CB	2.36	0.56
1:B:532:TYR:HE2	3:B:2074:HOH:O	1.87	0.55
1:D:598:ILE:HB	1:D:612:PHE:HB2	1.89	0.55
1:D:450:VAL:HG21	1:D:693:GLN:HG3	1.88	0.55
1:D:543:CYS:SG	1:D:544:THR:HG23	2.43	0.54
1:B:663:LEU:HD13	1:B:672:LEU:HD11	1.89	0.54
1:D:462:PRO:HD2	1:D:465:ALA:HB2	1.90	0.54
1:B:585:ASP:O	1:B:586:SER:HB2	2.07	0.54
1:D:646:ARG:HD3	3:D:2105:HOH:O	2.05	0.54
1:D:647:GLU:HB2	3:D:2103:HOH:O	2.06	0.54
1:C:723:ASN:ND2	1:C:735:GLN:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:678:SER:O	1:D:679:SER:CB	2.56	0.53
1:A:705:LYS:CE	3:A:2197:HOH:O	2.56	0.53
1:B:457:GLN:HG2	3:B:2017:HOH:O	2.08	0.53
1:C:454:GLY:HA3	1:C:455:GLN:HB3	1.83	0.53
1:B:513:SER:C	1:B:515:PRO:CD	2.70	0.53
1:C:451:THR:HG23	1:C:453:ASP:OD1	2.08	0.53
1:D:676:MET:CE	1:D:676:MET:CA	2.79	0.53
1:D:660:ILE:HA	1:D:676:MET:CE	2.39	0.52
1:D:543:CYS:HG	1:D:544:THR:HG22	1.69	0.52
1:A:585:ASP:O	1:A:586:SER:HB2	2.09	0.52
1:A:762:LYS:CE	3:A:2236:HOH:O	1.86	0.52
1:D:513:SER:O	1:D:514:HIS:O	2.28	0.52
1:B:529:ARG:HD3	3:B:2069:HOH:O	2.10	0.52
1:D:558:ASP:HB2	1:D:567:LYS:HD2	1.91	0.52
1:B:476:ARG:HH11	1:B:476:ARG:CG	2.22	0.51
1:D:576:ALA:HB3	1:D:594:SER:HB3	1.92	0.51
1:B:552:SER:HB2	3:B:2086:HOH:O	2.09	0.51
1:B:598:ILE:HB	1:B:612:PHE:HB2	1.91	0.51
1:D:563:THR:H	1:D:564:PRO:HD2	1.76	0.51
1:A:599:ALA:HB1	1:A:608:LEU:HD11	1.93	0.50
1:B:511:ASP:O	1:B:515:PRO:HG2	2.12	0.50
1:D:617:ASP:O	1:D:618:GLY:C	2.50	0.50
1:B:515:PRO:CD	1:B:516:GLY:N	2.74	0.50
1:B:612:PHE:CE1	1:B:648:GLY:HA2	2.47	0.50
1:D:503:GLY:C	3:D:2038:HOH:O	2.49	0.50
1:D:542:GLY:N	1:D:543:CYS:CB	2.67	0.50
1:C:716:THR:HB	1:C:742:VAL:CG1	2.42	0.50
1:A:604:HIS:HB3	3:A:2122:HOH:O	2.12	0.50
1:C:598:ILE:HB	1:C:612:PHE:HB2	1.93	0.50
1:B:610:ARG:HG3	1:B:611:GLN:N	2.27	0.50
1:D:486:VAL:HG13	1:D:743:LEU:CD2	2.41	0.49
1:D:631:LEU:HB2	1:D:645:LEU:HD21	1.94	0.49
1:A:631:LEU:HB2	1:A:645:LEU:HD21	1.94	0.49
1:C:723:ASN:ND2	1:C:735:GLN:HE21	2.08	0.49
1:C:604:HIS:CD2	3:C:2096:HOH:O	2.66	0.49
1:B:561:ALA:O	1:B:563:THR:N	2.45	0.49
2:X:2:MET:HA	2:X:2:MET:CE	2.43	0.49
1:B:534:ARG:NH1	1:B:550:GLU:OE2	2.42	0.49
1:C:604:HIS:HD2	3:C:2096:HOH:O	1.96	0.49
1:B:587:LYS:HG3	1:B:588:VAL:HG23	1.95	0.48
1:A:479:ASN:CB	3:A:2039:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:GLY:C	1:D:518:LYS:HB2	2.32	0.48
1:A:480:THR:HG23	1:A:762:LYS:HD3	1.96	0.48
1:A:550:GLU:CG	2:X:2:MET:HG2	2.43	0.48
1:D:652:GLN:HE22	1:D:687:ASN:ND2	2.10	0.48
1:B:498:HIS:HE1	3:B:2057:HOH:O	1.97	0.48
1:B:512:ILE:HA	1:B:516:GLY:HA2	1.96	0.48
1:D:486:VAL:CG1	1:D:743:LEU:CD2	2.89	0.48
1:D:515:PRO:HG3	1:D:517:ASN:HB2	1.94	0.48
1:D:515:PRO:CG	1:D:517:ASN:HB2	2.43	0.48
1:D:540:PRO:HA	3:D:2055:HOH:O	2.12	0.48
1:D:563:THR:N	1:D:564:PRO:CD	2.76	0.47
1:B:457:GLN:NE2	3:B:2017:HOH:O	2.39	0.47
1:D:625:SER:HB2	1:D:630:LYS:H	1.79	0.47
1:A:650:GLN:NE2	1:A:653:GLN:HB2	2.29	0.47
1:B:532:TYR:HB2	1:B:550:GLU:OE1	2.14	0.47
1:B:512:ILE:HA	1:B:516:GLY:CA	2.45	0.47
1:D:572:SER:HB2	3:D:2062:HOH:O	2.14	0.47
1:A:716:THR:HB	1:A:742:VAL:HB	1.97	0.47
1:A:529:ARG:HD2	3:A:2072:HOH:O	2.14	0.47
1:B:479:ASN:HA	1:B:517:ASN:OD1	2.15	0.47
1:C:615:HIS:CE1	1:C:641:ARG:HD2	2.50	0.47
1:C:451:THR:HG22	1:C:455:GLN:HB3	1.97	0.47
1:B:517:ASN:CA	1:B:518:LYS:HB3	2.30	0.47
1:C:604:HIS:HB3	3:C:2096:HOH:O	2.14	0.47
1:C:461:PHE:HB3	1:C:465:ALA:CB	2.44	0.47
1:B:572:SER:HB2	3:B:2091:HOH:O	2.14	0.46
1:A:688:LYS:HB3	1:A:689:PRO:CD	2.40	0.46
1:A:598:ILE:HB	1:A:612:PHE:HB2	1.98	0.46
1:D:597:ASN:ND2	3:D:2073:HOH:O	2.46	0.46
1:B:518:LYS:O	3:B:2060:HOH:O	2.21	0.46
1:B:456:MET:O	1:B:456:MET:HG2	2.16	0.46
1:A:483:HIS:HE1	3:A:2053:HOH:O	1.99	0.46
1:D:497:ARG:HD3	3:D:2085:HOH:O	2.14	0.46
1:B:517:ASN:HB3	1:B:518:LYS:HD3	1.98	0.46
1:B:541:ASP:C	1:B:541:ASP:OD1	2.55	0.46
1:A:461:PHE:HB3	1:A:465:ALA:CB	2.45	0.45
1:C:670:GLU:OE2	1:C:685:HIS:NE2	2.46	0.45
1:D:660:ILE:N	1:D:660:ILE:HD12	2.31	0.45
1:D:450:VAL:CG2	1:D:693:GLN:HG3	2.46	0.45
1:B:637:ASP:O	1:B:638:ASN:HB2	2.17	0.45
1:A:561:ALA:HB2	3:A:2090:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ARG:HG3	1:B:647:GLU:H	1.82	0.45
1:A:498:HIS:HE1	3:A:2056:HOH:O	2.00	0.45
1:A:527:LEU:HD13	1:A:531:ASN:HB2	1.97	0.45
1:D:563:THR:HG22	1:D:563:THR:O	2.17	0.44
1:D:612:PHE:HE1	1:D:648:GLY:HA2	1.82	0.44
1:A:662:SER:HB3	1:A:703:SER:HA	1.98	0.44
1:A:723:ASN:OD1	1:A:735:GLN:HG2	2.18	0.44
1:B:585:ASP:CG	1:B:587:LYS:HG2	2.37	0.44
1:A:546:ILE:HD12	1:A:582:ILE:HD12	1.99	0.44
1:B:479:ASN:CB	1:B:517:ASN:OD1	2.65	0.44
1:A:615:HIS:CE1	1:A:641:ARG:HD2	2.52	0.44
1:B:544:THR:CG2	1:B:556:ILE:HD12	2.48	0.44
1:D:528:ASN:HB3	1:D:531:ASN:HD22	1.81	0.44
1:D:625:SER:OG	1:D:630:LYS:HB2	2.18	0.44
1:D:666:CYS:HA	1:D:667:PRO:HD3	1.79	0.44
1:B:479:ASN:HB2	1:B:765:VAL:HB	1.99	0.43
1:B:476:ARG:HG2	1:B:476:ARG:HH11	1.83	0.43
1:C:437:GLN:HB3	1:D:461:PHE:CE2	2.53	0.43
1:B:515:PRO:HD2	1:B:516:GLY:N	2.32	0.43
1:A:451:THR:O	1:A:454:GLY:HA3	2.19	0.43
1:D:663:LEU:HA	1:D:673:ALA:O	2.18	0.43
1:B:631:LEU:HB3	1:B:643:TRP:HB2	2.00	0.43
1:D:660:ILE:HG13	1:D:676:MET:HE1	2.01	0.43
1:C:544:THR:HG21	3:C:2118:HOH:O	2.19	0.43
1:D:501:THR:O	1:D:507:VAL:HA	2.18	0.43
1:C:541:ASP:CG	3:C:2066:HOH:O	2.57	0.43
1:D:728:PRO:HD2	1:D:729:TYR:CD1	2.54	0.43
1:A:565:ARG:HD3	3:A:2090:HOH:O	2.19	0.43
1:A:498:HIS:HA	1:A:510:TRP:O	2.18	0.43
1:C:688:LYS:HB3	1:C:689:PRO:CD	2.49	0.43
1:B:544:THR:HG21	1:B:556:ILE:HD12	2.01	0.43
1:C:585:ASP:O	1:C:586:SER:HB2	2.19	0.43
1:C:716:THR:HB	1:C:742:VAL:HB	2.00	0.42
1:C:615:HIS:CE1	1:C:641:ARG:CD	3.02	0.42
1:C:498:HIS:HA	1:C:510:TRP:O	2.19	0.42
1:D:449:HIS:O	1:D:456:MET:HA	2.19	0.42
1:C:663:LEU:C	1:C:663:LEU:HD12	2.40	0.42
1:C:745:CYS:HA	1:C:755:VAL:O	2.19	0.42
1:D:539:LEU:HD12	1:D:544:THR:CG2	2.47	0.42
1:D:676:MET:HE2	1:D:676:MET:CA	2.46	0.42
1:D:598:ILE:HG12	1:D:633:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:617:ASP:HB2	3:D:2089:HOH:O	2.18	0.42
1:C:453:ASP:N	1:C:453:ASP:OD1	2.45	0.41
1:B:745:CYS:HA	1:B:755:VAL:O	2.20	0.41
2:Y:2:MET:HA	2:Y:2:MET:CE	2.50	0.41
1:D:686:VAL:O	1:D:687:ASN:HB2	2.20	0.41
1:A:646:ARG:HB2	1:A:646:ARG:HE	1.73	0.41
1:A:761:LYS:HD3	3:A:2237:HOH:O	2.21	0.41
1:C:561:ALA:C	1:C:563:THR:HA	2.38	0.41
1:B:580:LEU:HD22	1:B:589:CYS:SG	2.60	0.41
1:B:479:ASN:ND2	1:B:517:ASN:OD1	2.53	0.41
1:A:434:ASP:HA	3:A:2001:HOH:O	2.20	0.41
1:A:562:PRO:HB2	1:A:563:THR:H	1.75	0.41
1:C:685:HIS:HB3	1:C:688:LYS:HB2	2.03	0.41
1:C:546:ILE:HD12	1:C:582:ILE:CD1	2.51	0.41
1:D:541:ASP:C	1:D:543:CYS:CB	2.89	0.41
1:B:494:ASN:CG	1:B:749:VAL:HG21	2.40	0.41
1:D:585:ASP:O	1:D:586:SER:HB2	2.20	0.41
1:A:518:LYS:HE3	1:A:518:LYS:HA	2.02	0.41
1:C:504:LYS:HG3	1:C:532:TYR:CE1	2.56	0.41
1:B:676:MET:HG2	1:B:680:ASN:O	2.20	0.41
1:D:541:ASP:N	1:D:541:ASP:OD1	2.55	0.41
1:D:631:LEU:O	1:D:642:SER:HA	2.21	0.40
1:C:676:MET:HB2	1:C:680:ASN:O	2.21	0.40
1:D:602:ASP:HB2	1:D:609:VAL:HG11	2.03	0.40
1:A:550:GLU:HG2	2:X:2:MET:CG	2.49	0.40
1:C:660:ILE:HD12	1:C:676:MET:HE2	2.02	0.40
1:B:454:GLY:HA2	3:B:2015:HOH:O	2.21	0.40
1:A:705:LYS:NZ	3:A:2197:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/337 (99%)	325 (97%)	8 (2%)	2 (1%)	30 24
1	B	335/337 (99%)	313 (93%)	15 (4%)	7 (2%)	9 3
1	C	335/337 (99%)	319 (95%)	10 (3%)	6 (2%)	11 4
1	D	328/337 (97%)	302 (92%)	11 (3%)	15 (5%)	3 0
2	X	3/5 (60%)	3 (100%)	0	0	100 100
2	Y	3/5 (60%)	3 (100%)	0	0	100 100
All	All	1339/1358 (99%)	1265 (94%)	44 (3%)	30 (2%)	8 3

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	514	HIS
1	B	515	PRO
1	B	562	PRO
1	C	563	THR
1	D	514	HIS
1	D	515	PRO
1	D	543	CYS
1	D	562	PRO
1	D	625	SER
1	A	562	PRO
1	C	455	GLN
1	C	564	PRO
1	D	519	SER
1	D	560	ALA
1	D	618	GLY
1	A	497	ARG
1	B	497	ARG
1	B	516	GLY
1	B	679	SER
1	C	497	ARG
1	D	518	LYS
1	D	541	ASP
1	D	564	PRO
1	D	679	SER
1	C	679	SER
1	D	497	ARG
1	D	563	THR
1	D	561	ALA
1	C	562	PRO
1	B	542	GLY

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	288/288 (100%)	278 (96%)	10 (4%)	43 44
1	B	288/288 (100%)	274 (95%)	14 (5%)	31 27
1	C	288/288 (100%)	276 (96%)	12 (4%)	36 35
1	D	285/288 (99%)	269 (94%)	16 (6%)	26 22
2	X	5/5 (100%)	4 (80%)	1 (20%)	1 0
2	Y	5/5 (100%)	5 (100%)	0	100 100
All	All	1159/1162 (100%)	1106 (95%)	53 (5%)	33 30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	ASP
1	A	455	GLN
1	A	458	PRO
1	A	518	LYS
1	A	524	LEU
1	A	533	ILE
1	A	544	THR
1	A	663	LEU
1	A	676	MET
1	A	704	LEU
1	B	476	ARG
1	B	481	LEU
1	B	491	THR
1	B	514	HIS
1	B	515	PRO
1	B	518	LYS
1	B	556	ILE
1	B	567	LYS
1	B	609	VAL
1	B	610	ARG
1	B	663	LEU
1	B	676	MET

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Mol	Chain	Res	Type
1	B	677	GLU
1	B	743	LEU
1	C	447	SER
1	C	451	THR
1	C	453	ASP
1	C	467	ILE
1	C	519	SER
1	C	524	LEU
1	C	529	ARG
1	C	544	THR
1	C	660	ILE
1	C	663	LEU
1	C	676	MET
1	C	743	LEU
1	D	515	PRO
1	D	517	ASN
1	D	529	ARG
1	D	541	ASP
1	D	543	CYS
1	D	544	THR
1	D	565	ARG
1	D	597	ASN
1	D	617	ASP
1	D	625	SER
1	D	626	ASN
1	D	649	ARG
1	D	657	THR
1	D	658	SER
1	D	660	ILE
1	D	676	MET
2	X	2	MET

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	449	HIS
1	A	474	HIS
1	A	482	ASN
1	A	483	HIS
1	A	498	HIS
1	A	613	GLN
1	B	498	HIS

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Mol	Chain	Res	Type
1	B	528	ASN
1	B	611	GLN
1	B	680	ASN
1	B	695	HIS
1	C	531	ASN
1	C	613	GLN
1	C	654	HIS
1	C	695	HIS
1	C	723	ASN
1	D	482	ASN
1	D	514	HIS
1	D	531	ASN
1	D	626	ASN
1	D	687	ASN
1	D	695	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	337/337 (100%)	-0.30	3 (0%) 85 88	13, 20, 40, 57	0
1	B	337/337 (100%)	-0.10	9 (2%) 58 65	14, 23, 44, 57	0
1	C	337/337 (100%)	-0.28	4 (1%) 81 85	15, 23, 44, 57	0
1	D	332/337 (98%)	-0.05	11 (3%) 50 59	15, 25, 45, 59	0
2	X	5/5 (100%)	-0.10	0 100 100	28, 29, 34, 37	0
2	Y	5/5 (100%)	-0.07	0 100 100	31, 31, 37, 40	0
All	All	1353/1358 (99%)	-0.18	27 (1%) 68 73	13, 23, 44, 59	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	516	GLY	5.7
1	B	517	ASN	5.1
1	D	517	ASN	4.7
1	A	561	ALA	3.4
1	D	617	ASP	3.3
1	B	561	ALA	3.1
1	B	516	GLY	3.1
1	D	515	PRO	2.9
1	C	562	PRO	2.8
1	B	646	ARG	2.8
1	C	454	GLY	2.7
1	D	646	ARG	2.7
1	D	543	CYS	2.6
1	D	649	ARG	2.6
1	D	541	ASP	2.6
1	C	563	THR	2.5
1	A	452	ALA	2.5
1	B	562	PRO	2.5
1	A	434	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	456	MET	2.3
1	B	515	PRO	2.3
1	B	649	ARG	2.3
1	D	565	ARG	2.3
1	B	451	THR	2.2
1	C	434	ASP	2.2
1	B	647	GLU	2.1
1	D	529	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no 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.