Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:55 PM GMT

PDB ID	:	1MQS
Title	:	Crystal structure of Sly1p in complex with an N-terminal peptide of Sed5p
Authors	:	Bracher, A.; Weissenhorn, W.
Deposited on	:	2002-09-17
Resolution	:	3.00 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:

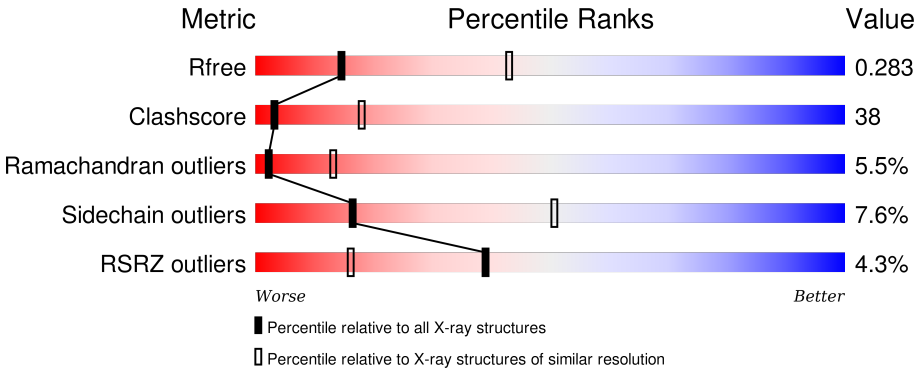
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	671	4%, 41%, 41%, 5% •, 12%
2	B	50	34%, 18%, 48%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4725 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 Sly1 Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	Se	0	0	0
			4506	2871	731	892	2	10			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P22213
A	-3	LYS	-	CLONING ARTIFACT	UNP P22213
A	-2	SER	-	CLONING ARTIFACT	UNP P22213
A	-1	ALA	-	CLONING ARTIFACT	UNP P22213
A	0	SER	-	CLONING ARTIFACT	UNP P22213
A	17	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	25	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	273	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	283	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	329	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	401	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	497	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	502	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	566	MSE	MET	MODIFIED RESIDUE	UNP P22213
A	637	MSE	MET	MODIFIED RESIDUE	UNP P22213

- Molecule 2 is a protein called Integral Membrane Protein SED5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	S	0	0	0
			199	122	38	38	1			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	CLONING ARTIFACT	UNP Q01590

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ALA	-	CLONING ARTIFACT	UNP Q01590
B	-2	MET	-	CLONING ARTIFACT	UNP Q01590
B	-1	ALA	-	CLONING ARTIFACT	UNP Q01590
B	0	GLY	-	CLONING ARTIFACT	UNP Q01590

- Molecule 3 is water.

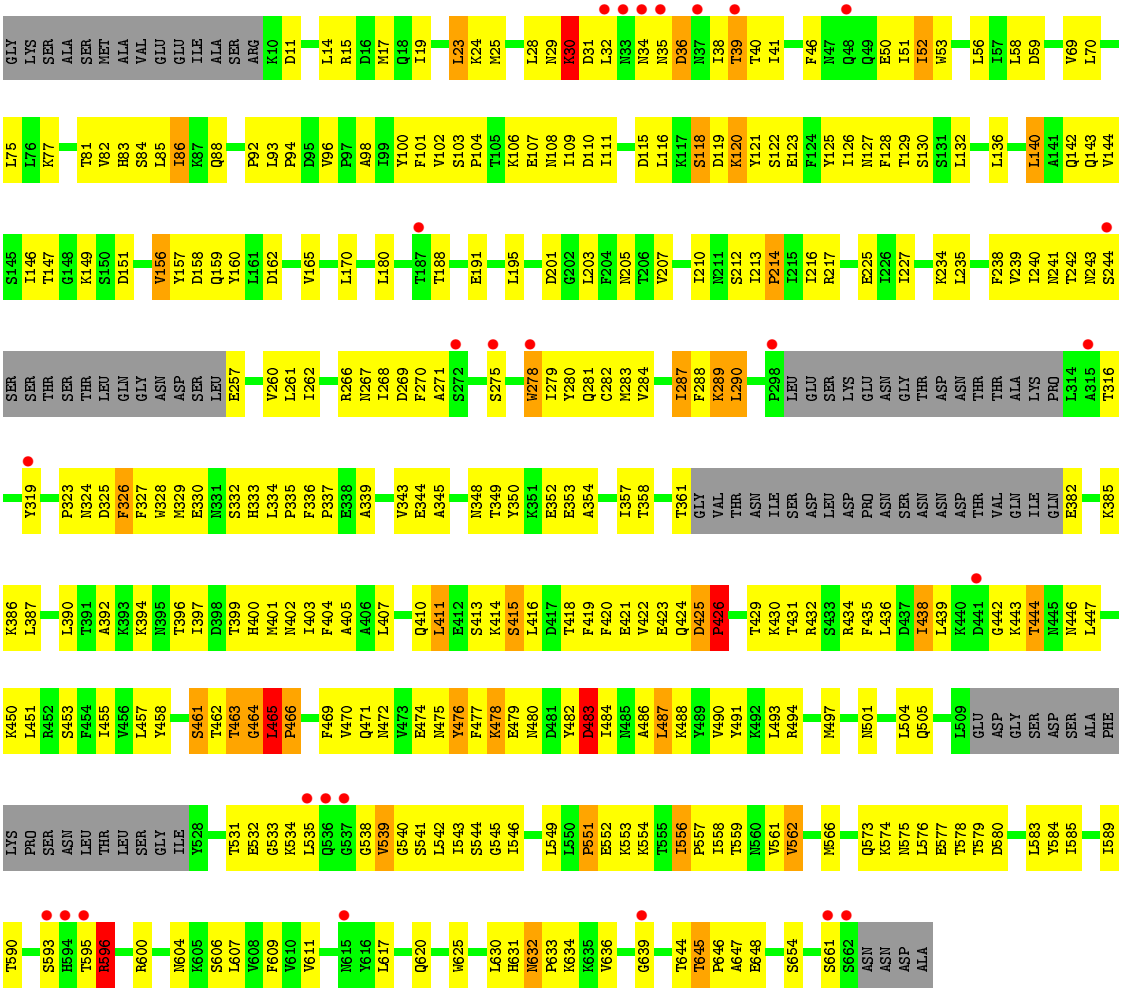
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	1	Total O 1 1	0	0

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.

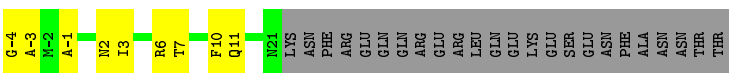
- Molecule 1: Sly1 Protein

Chain A:



- Molecule 2: Integral Membrane Protein SED5

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	161.06Å 161.06Å 88.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-3.00) 99.9 (29.91-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.290 0.255 , 0.283	Depositor DCC
R_{free} test set	1201 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	83.8	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 26122 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4725	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	0.46	1/4574 (0.0%)	0.74	2/6213 (0.0%)
2	B	0.44	0/200	0.63	0/264
All	All	0.45	1/4774 (0.0%)	0.74	2/6477 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	LYS	CA-CB	-6.12	1.40	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596	ARG	N-CA-C	-6.46	93.55	111.00
1	A	38	ILE	N-CA-C	-5.63	95.80	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4506	0	4353	345	0
2	B	199	0	199	10	0
3	A	19	0	0	2	0
3	B	1	0	0	0	0
All	All	4725	0	4552	348	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 38.

All (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HA	1:A:432:ARG:HB2	1.26	1.12
1:A:539:VAL:HG12	1:A:540:GLY:H	1.09	1.11
1:A:576:LEU:HD22	1:A:600:ARG:HH11	1.09	1.11
1:A:562:VAL:HG12	1:A:566:MSE:HE2	1.27	1.09
1:A:29:ASN:HB3	1:A:32:LEU:HD12	1.35	1.07
1:A:283:MSE:HE1	1:A:336:PHE:HB2	1.06	1.03
1:A:414:LYS:HE3	1:A:416:LEU:HD13	1.39	1.01
1:A:25:MSE:HE2	1:A:127:ASN:HB3	1.40	1.00
1:A:504:LEU:HD23	1:A:578:THR:HG21	1.42	1.00
1:A:24:LYS:HE2	1:A:32:LEU:HG	1.43	0.97
1:A:470:VAL:O	1:A:474:GLU:HB2	1.65	0.96
1:A:539:VAL:HG12	1:A:540:GLY:N	1.77	0.96
1:A:645:THR:HB	1:A:648:GLU:HG3	1.44	0.94
1:A:283:MSE:HE1	1:A:336:PHE:CB	1.97	0.94
1:A:539:VAL:CG1	1:A:540:GLY:H	1.81	0.94
1:A:216:ILE:HB	1:A:585:ILE:HG23	1.49	0.92
1:A:562:VAL:CG1	1:A:566:MSE:HE2	1.97	0.92
1:A:576:LEU:HD22	1:A:600:ARG:NH1	1.87	0.89
1:A:279:ILE:HD11	1:A:282:CYS:SG	2.13	0.88
1:A:539:VAL:HG13	1:A:543:ILE:HB	1.56	0.88
1:A:283:MSE:CE	1:A:336:PHE:HB2	2.00	0.87
1:A:52:ILE:HD13	1:A:52:ILE:H	1.39	0.87
1:A:283:MSE:O	1:A:287:ILE:HG12	1.74	0.87
1:A:327:PHE:CZ	1:A:343:VAL:HG23	2.10	0.86
1:A:158:ASP:OD2	2:B:6:ARG:HD2	1.76	0.86
1:A:539:VAL:HG12	1:A:541:SER:H	1.43	0.84
1:A:549:LEU:O	1:A:551:PRO:HD3	1.78	0.82
1:A:424:GLN:HE21	1:A:551:PRO:HG2	1.42	0.82
1:A:14:LEU:HA	1:A:17:MSE:HE3	1.62	0.81
1:A:266:ARG:O	1:A:266:ARG:HD3	1.81	0.81
1:A:261:LEU:HD12	1:A:607:LEU:HB3	1.63	0.80
1:A:25:MSE:HE2	1:A:127:ASN:CB	2.12	0.80
1:A:461:SER:O	1:A:462:THR:HG22	1.82	0.79
1:A:25:MSE:CE	1:A:127:ASN:HB3	2.13	0.79
1:A:235:LEU:O	1:A:239:VAL:HG23	1.83	0.78
1:A:336:PHE:HB3	1:A:337:PRO:HD3	1.64	0.78
1:A:278:TRP:O	1:A:283:MSE:HE2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PHE:CE1	1:A:407:LEU:HD23	2.19	0.78
1:A:418:THR:O	1:A:421:GLU:HG2	1.83	0.78
1:A:261:LEU:HD13	1:A:607:LEU:HD23	1.67	0.77
1:A:504:LEU:CD2	1:A:578:THR:HG21	2.15	0.77
1:A:556:ILE:HG23	1:A:557:PRO:HD2	1.68	0.75
1:A:29:ASN:HB3	1:A:32:LEU:CD1	2.14	0.74
1:A:104:PRO:HD3	1:A:129:THR:HG22	1.68	0.74
1:A:558:ILE:O	1:A:562:VAL:HG23	1.88	0.74
1:A:432:ARG:HB3	1:A:469:PHE:HZ	1.53	0.72
1:A:486:ALA:HB2	1:A:654:SER:HB3	1.72	0.72
1:A:539:VAL:HG12	1:A:541:SER:N	2.03	0.72
1:A:92:PRO:O	1:A:93:LEU:HD22	1.89	0.72
1:A:147:THR:HG22	1:A:149:LYS:H	1.54	0.72
1:A:109:ILE:HD11	1:A:132:LEU:HD11	1.71	0.71
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.25	0.70
1:A:201:ASP:OD1	1:A:234:LYS:HE2	1.91	0.70
1:A:589:ILE:HG22	1:A:590:THR:N	2.06	0.70
1:A:281:GLN:HG3	1:A:332:SER:O	1.91	0.70
1:A:213:ILE:HD13	1:A:239:VAL:HG22	1.71	0.70
1:A:278:TRP:HA	1:A:278:TRP:HE3	1.56	0.69
1:A:93:LEU:HD12	1:A:96:VAL:HG21	1.75	0.68
1:A:425:ASP:N	1:A:426:PRO:HD2	2.09	0.68
1:A:419:PHE:O	1:A:423:GLU:HG3	1.95	0.67
1:A:52:ILE:CD1	1:A:52:ILE:H	2.07	0.67
1:A:386:LYS:O	1:A:387:LEU:HD23	1.94	0.67
1:A:432:ARG:HD3	1:A:469:PHE:CE1	2.29	0.67
1:A:350:TYR:CE2	1:A:394:LYS:HG3	2.29	0.67
1:A:645:THR:CB	1:A:648:GLU:HG3	2.21	0.66
1:A:645:THR:HB	1:A:648:GLU:CG	2.22	0.65
1:A:425:ASP:HB3	1:A:431:THR:OG1	1.97	0.65
1:A:436:LEU:H	1:A:436:LEU:HD12	1.60	0.65
1:A:596:ARG:HG2	1:A:596:ARG:NH1	2.10	0.65
1:A:339:ALA:HB1	1:A:404:PHE:HZ	1.62	0.65
1:A:422:VAL:HG12	1:A:457:LEU:HD11	1.78	0.65
1:A:589:ILE:HG22	1:A:590:THR:H	1.60	0.65
1:A:350:TYR:CZ	1:A:394:LYS:HG3	2.32	0.65
1:A:35:ASN:O	1:A:36:ASP:HB2	1.95	0.65
1:A:84:SER:HB3	1:A:88:GLN:OE1	1.98	0.64
1:A:596:ARG:CG	1:A:596:ARG:HH11	2.09	0.64
1:A:288:PHE:CE1	1:A:407:LEU:HD12	2.32	0.64
1:A:458:TYR:CE2	1:A:491:TYR:HA	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:HA	1:A:432:ARG:CB	2.16	0.64
1:A:484:ILE:HG22	1:A:487:LEU:HB2	1.80	0.63
1:A:59:ASP:HB2	1:A:86:ILE:HD11	1.79	0.63
1:A:477:PHE:HB3	1:A:484:ILE:HD11	1.81	0.63
1:A:69:VAL:HG23	1:A:70:LEU:HD13	1.81	0.63
1:A:30:LYS:C	1:A:32:LEU:H	2.01	0.63
1:A:279:ILE:HD13	1:A:620:GLN:CG	2.28	0.63
1:A:270:PHE:CD2	1:A:493:LEU:HD13	2.34	0.63
1:A:436:LEU:HA	1:A:439:LEU:HG	1.79	0.63
1:A:596:ARG:HG2	1:A:596:ARG:HH11	1.64	0.63
1:A:556:ILE:HG23	1:A:557:PRO:CD	2.29	0.62
1:A:447:LEU:HG	1:A:482:TYR:CD2	2.35	0.62
1:A:573:GLN:O	1:A:577:GLU:HG3	1.99	0.62
1:A:59:ASP:CB	1:A:86:ILE:HD11	2.29	0.62
1:A:188:THR:HB	1:A:191:GLU:H	1.64	0.62
1:A:103:SER:HA	1:A:129:THR:HG22	1.82	0.62
1:A:132:LEU:O	2:B:6:ARG:NH1	2.33	0.62
1:A:279:ILE:HD13	1:A:620:GLN:HG2	1.80	0.62
1:A:53:TRP:HB3	1:A:81:THR:OG1	2.01	0.61
1:A:539:VAL:HG13	1:A:543:ILE:CB	2.28	0.61
1:A:561:VAL:HG13	1:A:579:THR:HG22	1.83	0.61
1:A:217:ARG:HD2	1:A:584:TYR:HA	1.83	0.61
1:A:432:ARG:HB3	1:A:469:PHE:CZ	2.33	0.61
1:A:420:PHE:O	1:A:424:GLN:HG2	2.01	0.61
1:A:280:TYR:O	1:A:284:VAL:HG23	2.02	0.60
1:A:336:PHE:HE1	1:A:407:LEU:HD23	1.67	0.60
1:A:81:THR:HG22	1:A:82:VAL:HG23	1.84	0.60
1:A:539:VAL:HG11	1:A:544:SER:H	1.66	0.59
1:A:325:ASP:O	1:A:327:PHE:N	2.35	0.59
1:A:576:LEU:CD2	1:A:600:ARG:HH11	2.01	0.59
1:A:556:ILE:HG22	1:A:558:ILE:HG22	1.84	0.59
1:A:631:HIS:O	1:A:632:ASN:HB2	2.02	0.59
1:A:267:ASN:HA	1:A:270:PHE:CE1	2.38	0.59
1:A:424:GLN:NE2	1:A:551:PRO:HG2	2.16	0.58
1:A:576:LEU:HB3	1:A:600:ARG:NH1	2.18	0.58
1:A:574:LYS:O	1:A:578:THR:HG22	2.04	0.58
1:A:348:ASN:O	1:A:352:GLU:HG2	2.04	0.58
1:A:140:LEU:HD13	2:B:10:PHE:CE1	2.38	0.58
2:B:7:THR:O	2:B:11:GLN:HG3	2.03	0.58
1:A:129:THR:HG23	1:A:130:SER:N	2.19	0.57
1:A:227:ILE:HD12	1:A:611:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PHE:O	1:A:289:LYS:C	2.43	0.57
1:A:458:TYR:HE2	1:A:491:TYR:HA	1.69	0.57
1:A:531:THR:C	1:A:533:GLY:N	2.57	0.57
1:A:25:MSE:HE3	1:A:159:GLN:OE1	2.04	0.57
1:A:397:ILE:O	1:A:401:MSE:HB2	2.04	0.57
1:A:484:ILE:HG22	1:A:484:ILE:O	2.04	0.57
1:A:566:MSE:HE1	1:A:636:VAL:CG2	2.35	0.57
1:A:210:ILE:CD1	1:A:607:LEU:HD22	2.34	0.57
1:A:238:PHE:HE2	2:B:-4:GLY:HA3	1.70	0.57
1:A:644:THR:HG23	1:A:648:GLU:HB2	1.87	0.56
1:A:243:ASN:O	1:A:244:SER:HB2	2.04	0.56
1:A:630:LEU:O	1:A:631:HIS:HB2	2.06	0.56
1:A:281:GLN:HE21	1:A:620:GLN:NE2	2.03	0.56
1:A:358:THR:HA	3:A:673:HOH:O	2.04	0.56
1:A:279:ILE:HD13	1:A:620:GLN:CD	2.27	0.56
1:A:106:LYS:HE3	1:A:110:ASP:OD2	2.05	0.56
1:A:103:SER:HA	1:A:129:THR:CG2	2.37	0.55
1:A:494:ARG:HG3	1:A:494:ARG:HH11	1.71	0.55
1:A:279:ILE:CD1	1:A:282:CYS:SG	2.93	0.55
1:A:19:ILE:HG12	1:A:69:VAL:HB	1.87	0.55
1:A:56:LEU:O	1:A:83:HIS:HA	2.07	0.55
1:A:271:ALA:HB2	1:A:497:MSE:HE2	1.88	0.55
1:A:323:PRO:O	1:A:324:ASN:HB2	2.06	0.55
1:A:93:LEU:N	1:A:94:PRO:HD3	2.23	0.54
1:A:25:MSE:HE1	1:A:101:PHE:CD1	2.42	0.54
1:A:401:MSE:HE3	1:A:401:MSE:HA	1.89	0.54
1:A:425:ASP:N	1:A:426:PRO:CD	2.70	0.54
1:A:645:THR:HG22	1:A:647:ALA:N	2.23	0.54
1:A:160:TYR:HA	1:A:205:ASN:ND2	2.22	0.54
1:A:461:SER:OG	1:A:494:ARG:NH1	2.41	0.54
1:A:147:THR:HG22	1:A:149:LYS:N	2.22	0.54
1:A:425:ASP:O	1:A:426:PRO:C	2.46	0.54
1:A:25:MSE:HE3	1:A:159:GLN:CD	2.27	0.54
1:A:461:SER:O	1:A:462:THR:CG2	2.56	0.53
1:A:34:ASN:CG	1:A:35:ASN:H	2.09	0.53
1:A:25:MSE:HE3	1:A:159:GLN:CG	2.39	0.53
1:A:100:TYR:O	1:A:127:ASN:HB2	2.08	0.53
1:A:69:VAL:O	1:A:70:LEU:HD12	2.07	0.53
1:A:278:TRP:C	1:A:283:MSE:HE2	2.28	0.53
1:A:19:ILE:HG23	1:A:70:LEU:HD11	1.91	0.53
1:A:216:ILE:HB	1:A:585:ILE:CG2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:CD1	1:A:620:GLN:HG2	2.38	0.53
1:A:539:VAL:HG13	1:A:543:ILE:H	1.72	0.53
1:A:645:THR:HG22	1:A:647:ALA:H	1.73	0.53
1:A:392:ALA:O	1:A:396:THR:HG23	2.09	0.53
1:A:28:LEU:HD13	1:A:125:TYR:CZ	2.44	0.53
1:A:539:VAL:HG21	1:A:544:SER:OG	2.09	0.52
1:A:207:VAL:HA	1:A:210:ILE:HD12	1.91	0.52
1:A:358:THR:O	1:A:358:THR:HG22	2.09	0.52
1:A:403:ILE:O	1:A:407:LEU:HB2	2.08	0.52
1:A:419:PHE:HE2	1:A:450:LYS:HA	1.74	0.52
1:A:354:ALA:CB	1:A:390:LEU:HD21	2.40	0.52
1:A:539:VAL:CG1	1:A:540:GLY:N	2.48	0.52
1:A:343:VAL:HG12	1:A:344:GLU:N	2.25	0.52
1:A:316:THR:O	1:A:316:THR:HG23	2.08	0.52
1:A:463:THR:O	1:A:463:THR:HG23	2.09	0.52
1:A:39:THR:O	1:A:39:THR:CG2	2.57	0.52
1:A:128:PHE:CE1	1:A:132:LEU:HD22	2.46	0.51
1:A:533:GLY:O	1:A:535:LEU:N	2.33	0.51
1:A:539:VAL:HG11	1:A:544:SER:OG	2.10	0.51
1:A:418:THR:OG1	1:A:419:PHE:N	2.44	0.51
1:A:435:PHE:O	1:A:438:ILE:HG22	2.10	0.51
1:A:576:LEU:HB3	1:A:600:ARG:HH12	1.75	0.51
1:A:633:PRO:O	1:A:634:LYS:HD3	2.10	0.51
1:A:24:LYS:HE2	1:A:32:LEU:CG	2.30	0.51
1:A:589:ILE:CG2	1:A:590:THR:N	2.75	0.51
1:A:344:GLU:OE2	1:A:532:GLU:O	2.29	0.50
1:A:238:PHE:CE2	2:B:-4:GLY:HA3	2.45	0.50
1:A:288:PHE:O	1:A:290:LEU:N	2.45	0.50
1:A:102:VAL:HG12	1:A:103:SER:N	2.27	0.50
1:A:464:GLY:O	1:A:465:LEU:CB	2.60	0.50
1:A:283:MSE:HB3	1:A:287:ILE:HD11	1.93	0.50
1:A:58:LEU:O	1:A:85:LEU:HA	2.12	0.50
1:A:484:ILE:HG21	1:A:487:LEU:HD12	1.93	0.50
1:A:339:ALA:HB1	1:A:404:PHE:CZ	2.44	0.50
1:A:327:PHE:CD2	1:A:400:HIS:CD2	3.01	0.49
1:A:25:MSE:HE2	1:A:127:ASN:CG	2.32	0.49
1:A:589:ILE:CG2	1:A:590:THR:H	2.26	0.49
1:A:29:ASN:O	1:A:32:LEU:HB2	2.13	0.49
1:A:432:ARG:HE	1:A:466:PRO:HD2	1.78	0.49
1:A:645:THR:HG22	1:A:647:ALA:HB3	1.95	0.49
1:A:109:ILE:CD1	1:A:136:LEU:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:H	1:A:205:ASN:ND2	2.11	0.49
1:A:575:ASN:HA	1:A:578:THR:CG2	2.43	0.48
1:A:86:ILE:HG12	1:A:108:ASN:ND2	2.28	0.48
1:A:477:PHE:CB	1:A:484:ILE:HD11	2.42	0.48
1:A:270:PHE:CZ	1:A:493:LEU:HD22	2.49	0.48
1:A:562:VAL:HG12	1:A:566:MSE:CE	2.19	0.48
1:A:325:ASP:HB3	1:A:328:TRP:HB3	1.95	0.48
1:A:432:ARG:HH21	1:A:466:PRO:HD3	1.77	0.48
1:A:472:ASN:HA	1:A:475:ASN:HD22	1.77	0.48
1:A:281:GLN:HE21	1:A:620:GLN:HE21	1.62	0.48
1:A:482:TYR:O	1:A:483:ASP:C	2.52	0.48
1:A:225:GLU:HG3	1:A:583:LEU:HD22	1.96	0.48
1:A:262:ILE:HD12	1:A:562:VAL:HG13	1.95	0.47
1:A:281:GLN:NE2	1:A:620:GLN:HE21	2.12	0.47
1:A:69:VAL:C	1:A:70:LEU:HD12	2.35	0.47
1:A:39:THR:HG23	1:A:39:THR:O	2.13	0.47
1:A:539:VAL:HG13	1:A:543:ILE:N	2.29	0.47
1:A:30:LYS:O	1:A:32:LEU:N	2.47	0.47
1:A:261:LEU:CD1	1:A:607:LEU:HB3	2.37	0.47
1:A:455:ILE:HD13	1:A:490:VAL:HG21	1.97	0.47
1:A:240:ILE:O	1:A:242:THR:N	2.38	0.47
1:A:575:ASN:HA	1:A:578:THR:HG22	1.96	0.47
1:A:86:ILE:HD12	1:A:86:ILE:N	2.30	0.47
1:A:319:TYR:CD2	1:A:399:THR:HG23	2.48	0.47
2:B:-1:ALA:O	2:B:2:ASN:HB2	2.14	0.47
1:A:278:TRP:NE1	1:A:546:ILE:HG23	2.30	0.47
1:A:162:ASP:H	1:A:205:ASN:HD22	1.62	0.47
1:A:644:THR:CG2	1:A:648:GLU:HB2	2.45	0.47
1:A:213:ILE:CD1	1:A:239:VAL:HG22	2.41	0.47
1:A:631:HIS:O	1:A:632:ASN:CB	2.63	0.47
1:A:242:THR:HG22	1:A:243:ASN:ND2	2.29	0.47
1:A:609:PHE:HA	1:A:639:GLY:O	2.15	0.47
1:A:129:THR:CG2	1:A:130:SER:N	2.77	0.47
1:A:396:THR:O	1:A:399:THR:HB	2.15	0.47
1:A:645:THR:HG23	1:A:646:PRO:HD2	1.96	0.46
1:A:462:THR:O	1:A:463:THR:HB	2.14	0.46
1:A:102:VAL:CG1	1:A:103:SER:N	2.77	0.46
1:A:104:PRO:HD3	1:A:129:THR:CG2	2.41	0.46
1:A:115:ASP:OD1	1:A:120:LYS:HE2	2.15	0.46
1:A:484:ILE:CG2	1:A:487:LEU:HD12	2.45	0.46
1:A:349:THR:O	1:A:353:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:THR:C	1:A:446:ASN:H	2.19	0.46
1:A:645:THR:CG2	1:A:647:ALA:HB3	2.46	0.46
1:A:140:LEU:HD22	1:A:144:VAL:HG23	1.98	0.46
1:A:410:GLN:O	1:A:414:LYS:HG2	2.15	0.46
1:A:217:ARG:HA	1:A:217:ARG:HD2	1.79	0.45
1:A:354:ALA:HB1	1:A:390:LEU:HD21	1.96	0.45
1:A:107:GLU:O	1:A:111:ILE:HG13	2.16	0.45
1:A:645:THR:CG2	1:A:647:ALA:H	2.29	0.45
1:A:29:ASN:C	1:A:30:LYS:O	2.54	0.45
1:A:156:VAL:HG13	2:B:7:THR:HA	1.99	0.45
1:A:126:ILE:O	1:A:156:VAL:HA	2.16	0.45
1:A:212:SER:O	1:A:214:PRO:HD3	2.16	0.45
1:A:382:GLU:N	3:A:684:HOH:O	2.49	0.45
1:A:541:SER:O	1:A:542:LEU:HD23	2.17	0.45
1:A:160:TYR:HA	1:A:205:ASN:HD21	1.81	0.45
1:A:539:VAL:CG1	1:A:541:SER:H	2.22	0.45
1:A:336:PHE:CD1	1:A:407:LEU:HD23	2.51	0.45
1:A:486:ALA:O	1:A:488:LYS:N	2.49	0.45
1:A:217:ARG:HG3	1:A:217:ARG:NH1	2.32	0.45
1:A:281:GLN:NE2	1:A:620:GLN:NE2	2.65	0.45
1:A:419:PHE:HB3	1:A:453:SER:OG	2.17	0.45
1:A:240:ILE:C	1:A:242:THR:H	2.18	0.45
1:A:538:GLY:C	1:A:539:VAL:HG23	2.38	0.45
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.82	0.44
1:A:217:ARG:CD	1:A:584:TYR:HA	2.46	0.44
1:A:41:ILE:H	1:A:41:ILE:HG13	1.37	0.44
1:A:104:PRO:HG2	1:A:130:SER:OG	2.17	0.44
1:A:201:ASP:OD1	1:A:234:LYS:CE	2.61	0.44
1:A:30:LYS:C	1:A:32:LEU:N	2.69	0.44
1:A:566:MSE:HE1	1:A:636:VAL:HG22	1.98	0.44
1:A:419:PHE:HD2	1:A:453:SER:OG	2.01	0.44
1:A:118:SER:O	1:A:119:ASP:HB2	2.17	0.44
1:A:439:LEU:HD12	1:A:439:LEU:C	2.38	0.44
1:A:477:PHE:CG	1:A:484:ILE:HD11	2.52	0.44
1:A:451:LEU:O	1:A:455:ILE:HG13	2.17	0.44
1:A:429:THR:O	1:A:430:LYS:C	2.55	0.44
1:A:29:ASN:O	1:A:32:LEU:HD12	2.18	0.44
1:A:345:ALA:O	1:A:349:THR:HG23	2.18	0.44
1:A:19:ILE:CG1	1:A:69:VAL:HB	2.48	0.44
1:A:122:SER:O	1:A:123:GLU:HG3	2.17	0.44
1:A:116:LEU:O	1:A:116:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TRP:C	1:A:330:GLU:H	2.20	0.43
1:A:102:VAL:HG11	1:A:108:ASN:CG	2.38	0.43
1:A:558:ILE:HG23	1:A:559:THR:N	2.33	0.43
1:A:32:LEU:HD13	1:A:157:TYR:OH	2.18	0.43
1:A:15:ARG:HB2	1:A:165:VAL:HG11	1.99	0.43
1:A:268:ILE:HG12	1:A:268:ILE:O	2.17	0.43
1:A:25:MSE:HE3	1:A:159:GLN:HG2	1.99	0.43
1:A:556:ILE:HG23	1:A:557:PRO:N	2.33	0.43
1:A:539:VAL:HG11	1:A:544:SER:N	2.32	0.43
1:A:438:ILE:O	1:A:438:ILE:HD13	2.19	0.43
1:A:343:VAL:HG11	1:A:401:MSE:CE	2.49	0.43
1:A:422:VAL:HG11	1:A:435:PHE:HD1	1.83	0.43
1:A:143:GLN:O	1:A:146:ILE:HG12	2.18	0.43
1:A:354:ALA:O	1:A:358:THR:OG1	2.20	0.43
1:A:46:PHE:CE2	1:A:51:ILE:HB	2.54	0.43
1:A:414:LYS:O	1:A:415:SER:C	2.57	0.43
1:A:471:GLN:O	1:A:475:ASN:ND2	2.52	0.43
1:A:257:GLU:N	1:A:604:ASN:HD21	2.17	0.43
1:A:279:ILE:HD13	1:A:620:GLN:NE2	2.34	0.42
1:A:386:LYS:C	1:A:387:LEU:HD23	2.40	0.42
1:A:402:ASN:HA	1:A:405:ALA:HB3	2.01	0.42
1:A:552:GLU:O	1:A:554:LYS:N	2.50	0.42
1:A:158:ASP:OD2	2:B:6:ARG:CD	2.59	0.42
1:A:447:LEU:HG	1:A:482:TYR:CE2	2.54	0.42
2:B:7:THR:O	2:B:10:PHE:HB3	2.19	0.42
1:A:290:LEU:HD22	1:A:290:LEU:C	2.40	0.42
1:A:344:GLU:O	1:A:348:ASN:HB2	2.19	0.42
1:A:385:LYS:HD3	1:A:386:LYS:H	1.84	0.42
1:A:35:ASN:O	1:A:36:ASP:CB	2.65	0.42
1:A:15:ARG:CB	1:A:165:VAL:HG11	2.50	0.42
1:A:279:ILE:HA	1:A:335:PRO:HA	2.01	0.42
1:A:334:LEU:HA	1:A:335:PRO:HD3	1.88	0.42
1:A:486:ALA:C	1:A:488:LYS:H	2.21	0.42
1:A:288:PHE:CE1	1:A:407:LEU:CD1	3.01	0.42
1:A:333:HIS:CE1	1:A:334:LEU:HD13	2.54	0.42
1:A:327:PHE:HB3	1:A:400:HIS:CD2	2.54	0.42
1:A:439:LEU:HB2	1:A:476:TYR:CE2	2.54	0.42
1:A:484:ILE:CG2	1:A:487:LEU:HB2	2.48	0.42
1:A:645:THR:O	1:A:646:PRO:C	2.58	0.42
1:A:436:LEU:HA	1:A:439:LEU:CG	2.46	0.42
1:A:463:THR:O	1:A:465:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:H	1:A:426:PRO:CD	2.32	0.41
1:A:556:ILE:CG2	1:A:558:ILE:HG22	2.49	0.41
1:A:102:VAL:CG1	1:A:108:ASN:CG	2.89	0.41
1:A:584:TYR:O	1:A:596:ARG:HB3	2.20	0.41
1:A:188:THR:OG1	1:A:191:GLU:HG3	2.20	0.41
1:A:461:SER:O	1:A:463:THR:HG22	2.20	0.41
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.70	0.41
1:A:566:MSE:HE3	1:A:625:TRP:CH2	2.55	0.41
1:A:566:MSE:SE	1:A:606:SER:HB3	2.70	0.41
1:A:260:VAL:O	1:A:606:SER:HA	2.21	0.41
1:A:545:GLY:O	1:A:549:LEU:HG	2.21	0.41
1:A:478:LYS:H	1:A:478:LYS:HG2	1.69	0.41
1:A:432:ARG:CB	1:A:469:PHE:CZ	3.03	0.41
1:A:270:PHE:CE2	1:A:493:LEU:HD13	2.56	0.41
1:A:497:MSE:O	1:A:501:ASN:HB2	2.21	0.41
1:A:539:VAL:CG1	1:A:544:SER:H	2.32	0.41
1:A:479:GLU:HG3	1:A:480:ASN:N	2.36	0.40
1:A:411:LEU:HD12	1:A:411:LEU:C	2.41	0.40
1:A:85:LEU:HB2	1:A:88:GLN:HG3	2.03	0.40
1:A:323:PRO:O	1:A:324:ASN:CB	2.69	0.40
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.89	0.40
1:A:539:VAL:CG1	1:A:543:ILE:H	2.35	0.40
1:A:357:ILE:HG21	1:A:387:LEU:HD13	2.02	0.40
1:A:98:ALA:HB2	1:A:121:TYR:CG	2.57	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	578/671 (86%)	467 (81%)	79 (14%)	32 (6%)	2 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	24/50 (48%)	20 (83%)	3 (12%)	1 (4%)	3 20
All	All	602/721 (84%)	487 (81%)	82 (14%)	33 (6%)	2 13

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	ASP
1	A	36	ASP
1	A	275	SER
1	A	326	PHE
1	A	426	PRO
1	A	442	GLY
1	A	461	SER
1	A	464	GLY
1	A	534	LYS
1	A	40	THR
1	A	289	LYS
2	B	-3	ALA
1	A	50	GLU
1	A	241	ASN
1	A	415	SER
1	A	434	ARG
1	A	444	THR
1	A	463	THR
1	A	483	ASP
1	A	487	LEU
1	A	593	SER
1	A	118	SER
1	A	269	ASP
1	A	413	SER
1	A	443	LYS
1	A	465	LEU
1	A	425	ASP
1	A	551	PRO
1	A	466	PRO
1	A	476	TYR
1	A	539	VAL
1	A	632	ASN

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	491/597 (82%)	453 (92%)	38 (8%)	16 50
2	B	20/45 (44%)	19 (95%)	1 (5%)	30 70
All	All	511/642 (80%)	472 (92%)	39 (8%)	16 51

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	23	LEU
1	A	39	THR
1	A	52	ILE
1	A	75	LEU
1	A	77	LYS
1	A	86	ILE
1	A	120	LYS
1	A	140	LEU
1	A	142	GLN
1	A	151	ASP
1	A	156	VAL
1	A	170	LEU
1	A	180	LEU
1	A	195	LEU
1	A	214	PRO
1	A	278	TRP
1	A	287	ILE
1	A	290	LEU
1	A	326	PHE
1	A	329	MSE
1	A	361	THR
1	A	411	LEU
1	A	426	PRO
1	A	438	ILE
1	A	465	LEU
1	A	478	LYS

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Mol	Chain	Res	Type
1	A	483	ASP
1	A	505	GLN
1	A	553	LYS
1	A	556	ILE
1	A	562	VAL
1	A	580	ASP
1	A	595	THR
1	A	596	ARG
1	A	617	LEU
1	A	645	THR
1	A	661	SER
2	B	3	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	108	ASN
1	A	205	ASN
1	A	243	ASN
1	A	276	HIS
1	A	342	ASN
1	A	402	ASN
1	A	424	GLN
1	A	620	GLN
1	A	621	ASN
1	A	632	ASN

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	578/671 (86%)	0.08	26 (4%) 37 15	57, 94, 159, 177	0
2	B	26/50 (52%)	-0.19	0 100 100	67, 81, 138, 145	0
All	All	604/721 (83%)	0.07	26 (4%) 39 16	57, 94, 159, 177	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	ASN	8.1
1	A	33	ASN	7.3
1	A	595	THR	6.0
1	A	594	HIS	4.4
1	A	244	SER	3.6
1	A	187	THR	3.3
1	A	32	LEU	3.2
1	A	593	SER	3.2
1	A	48	GLN	3.1
1	A	39	THR	3.1
1	A	615	ASN	3.0
1	A	278	TRP	3.0
1	A	35	ASN	3.0
1	A	37	ASN	2.9
1	A	298	PRO	2.8
1	A	319	TYR	2.7
1	A	661	SER	2.7
1	A	536	GLN	2.6
1	A	662	SER	2.5
1	A	639	GLY	2.5
1	A	272	SER	2.3
1	A	315	ALA	2.3
1	A	537	GLY	2.3
1	A	441	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	535	LEU	2.1
1	A	275	SER	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.