



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:56 AM UTC

PDB ID : 8PK5 / pdb_00008pk5
Title : INTS13-INTS14 complex with ZNF609
Authors : Sabath, K.; Jonas, S.
Deposited on : 2023-06-25
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

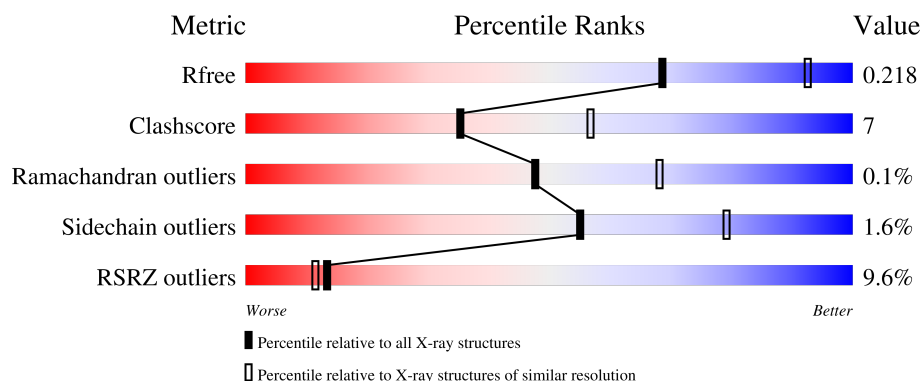
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	718	
2	B	538	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	B	600	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8017 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 Integrator complex subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4177	2614	736	795	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLY	-	expression tag	UNP Q9NVM9
A	-10	PRO	-	expression tag	UNP Q9NVM9
A	-9	SER	-	expression tag	UNP Q9NVM9
A	-8	ASP	-	expression tag	UNP Q9NVM9
A	-7	PRO	-	expression tag	UNP Q9NVM9
A	-6	GLY	-	expression tag	UNP Q9NVM9
A	-5	PRO	-	expression tag	UNP Q9NVM9
A	-4	LYS	-	expression tag	UNP Q9NVM9
A	-3	ARG	-	expression tag	UNP Q9NVM9
A	-2	ALA	-	expression tag	UNP Q9NVM9
A	-1	GLU	-	expression tag	UNP Q9NVM9
A	0	PHE	-	expression tag	UNP Q9NVM9

- Molecule 2 is a protein called Integrator complex subunit 14,Zinc finger protein 609.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	495	Total	C	N	O	S	0	0	0
			3790	2427	623	715	25			

There are 3 discrepancies between the modelled and reference sequences:

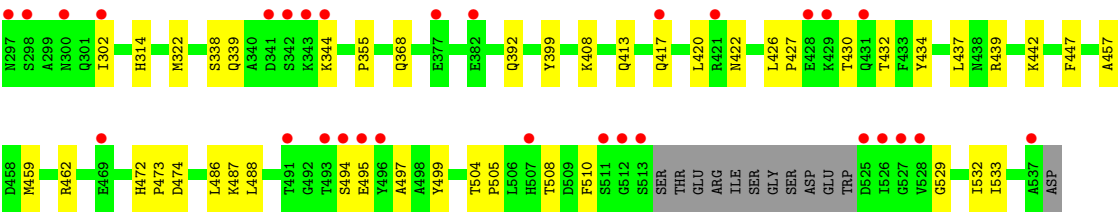
Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	-	linker	UNP Q96SY0
B	520	GLY	-	linker	UNP Q96SY0
B	521	SER	-	linker	UNP Q96SY0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	29	Total 29	O 29	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	189.06Å 115.63Å 147.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.50 47.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.94-2.50) 100.0 (47.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.190 , 0.214 0.196 , 0.218	Depositor DCC
R_{free} test set	5581 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8017	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.34	0/4259	0.55	0/5780
2	B	0.40	0/3873	0.61	0/5271
All	All	0.37	0/8132	0.58	0/11051

There are no bond length outliers.

There are no bond angle outliers.

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	4177	0	4082	64	0
2	B	3790	0	3737	59	0
3	B	1	0	0	0	0
4	A	20	0	0	0	0
4	B	29	0	0	1	0
All	All	8017	0	7819	117	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 7.

All (117) 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:147:LEU:HB3	1:A:151:ALA:HB3	1.57	0.85
1:A:267:MET:HE1	1:A:346:PRO:HA	1.59	0.84
2:B:63:MET:HE3	2:B:76:ALA:HB1	1.64	0.79
1:A:136:ILE:HD13	1:A:141:HIS:HB2	1.63	0.78
2:B:339:GLN:HE21	2:B:344:LYS:HB2	1.48	0.78
1:A:530:ARG:HD2	1:A:564:PRO:HG3	1.67	0.77
1:A:464:SER:HB3	1:A:516:VAL:HB	1.66	0.76
2:B:439:ARG:NH2	4:B:701:HOH:O	2.21	0.74
1:A:537:GLU:OE1	1:A:541:ARG:NH1	2.23	0.71
1:A:3:ILE:HD12	1:A:73:LYS:HE3	1.74	0.69
2:B:339:GLN:HE22	2:B:344:LYS:HD2	1.60	0.67
2:B:155:MET:HE3	2:B:200:MET:HE3	1.76	0.67
2:B:93:VAL:HG23	2:B:143:PRO:HG3	1.77	0.66
2:B:339:GLN:NE2	2:B:344:LYS:HB2	2.16	0.60
2:B:422:ASN:ND2	2:B:432:THR:OG1	2.33	0.59
2:B:474:ASP:OD1	2:B:508:THR:OG1	2.14	0.58
1:A:166:ALA:HB3	1:A:218:VAL:HG21	1.85	0.57
1:A:130:VAL:HG11	1:A:182:THR:HG22	1.87	0.57
2:B:61:GLU:HB2	2:B:85:LYS:HA	1.85	0.56
1:A:419:GLY:HA2	1:A:422:MET:HE2	1.86	0.56
1:A:61:GLU:OE2	1:A:64:ARG:NH2	2.38	0.56
1:A:353:PHE:CZ	1:A:358:ARG:HG2	2.41	0.56
1:A:354:LEU:HD21	1:A:360:VAL:HG12	1.88	0.55
2:B:473:PRO:HB2	2:B:510:PHE:CZ	2.42	0.55
1:A:318:TRP:HE1	1:A:320:THR:HG22	1.73	0.55
2:B:339:GLN:NE2	2:B:344:LYS:HD2	2.22	0.55
1:A:261:THR:HG22	1:A:282:GLU:HB2	1.89	0.54
1:A:227:SER:HB3	1:A:230:LEU:H	1.72	0.54
2:B:57:SER:OG	2:B:58:SER:N	2.38	0.54
2:B:413:GLN:O	2:B:417:GLN:HG2	2.08	0.54
1:A:79:ILE:HG12	1:A:87:VAL:HG12	1.89	0.54
1:A:180:GLN:HE21	1:A:227:SER:HB2	1.73	0.53
2:B:427:PRO:HD3	2:B:472:HIS:HB3	1.90	0.53
1:A:165:ASN:ND2	1:A:209:THR:O	2.41	0.53
2:B:157:MET:CE	2:B:200:MET:HE1	2.39	0.53
1:A:15:ASP:O	1:A:20:MET:HG3	2.10	0.52
2:B:427:PRO:O	2:B:430:THR:HG23	2.10	0.52
1:A:64:ARG:NH1	1:A:339:PRO:O	2.43	0.51
2:B:533:ILE:HD12	2:B:533:ILE:N	2.25	0.51
2:B:437:LEU:HD11	2:B:486:LEU:HD22	1.93	0.51
2:B:442:LYS:HE3	2:B:499:TYR:O	2.11	0.50
2:B:426:LEU:HD22	2:B:430:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG23	1:A:162:CYS:HA	1.93	0.49
1:A:467:THR:OG1	1:A:513:ILE:HG22	2.13	0.48
2:B:63:MET:HE1	2:B:80:MET:HB3	1.96	0.48
2:B:532:ILE:HG12	2:B:533:ILE:H	1.79	0.48
1:A:70:PHE:HB3	1:A:74:LYS:HG3	1.95	0.48
1:A:112:ASN:ND2	1:A:115:ALA:HB2	2.28	0.48
1:A:73:LYS:HG3	1:A:139:TYR:CE1	2.49	0.48
2:B:268:LEU:HD11	2:B:355:PRO:HD3	1.96	0.48
2:B:63:MET:HE1	2:B:80:MET:HE3	1.96	0.47
2:B:62:LEU:HD13	2:B:98:ILE:HD13	1.95	0.47
1:A:144:ARG:HG3	1:A:154:VAL:HG21	1.97	0.47
2:B:61:GLU:HG2	2:B:83:TYR:HE2	1.80	0.47
1:A:524:LYS:HD3	1:A:525:ARG:N	2.30	0.47
1:A:82:ASP:C	1:A:120:CYS:HB2	2.40	0.46
1:A:281:VAL:HG13	1:A:347:SER:HB2	1.98	0.46
1:A:563:LYS:HB2	1:A:563:LYS:HE2	1.60	0.46
2:B:61:GLU:HG2	2:B:83:TYR:CE2	2.50	0.46
1:A:61:GLU:CD	1:A:64:ARG:NH2	2.74	0.46
1:A:318:TRP:HE1	1:A:320:THR:CG2	2.29	0.46
2:B:228:PHE:CD1	2:B:229:PRO:HA	2.51	0.46
2:B:457:ALA:CB	2:B:487:LYS:HG3	2.47	0.45
2:B:495:GLU:C	2:B:497:ALA:H	2.22	0.45
1:A:68:ASP:HB2	1:A:338:SER:HB2	1.99	0.45
1:A:21:ALA:HB2	1:A:111:PRO:HG2	1.99	0.45
2:B:25:TYR:HB3	2:B:29:HIS:HB2	1.98	0.45
1:A:210:TYR:CE1	1:A:216:SER:HB3	2.51	0.45
1:A:154:VAL:HG23	1:A:197:MET:HE1	1.98	0.45
2:B:262:ILE:HG23	2:B:265:PRO:HD3	1.99	0.45
1:A:208:HIS:CD2	1:A:218:VAL:HB	2.52	0.45
1:A:351:THR:HG21	2:B:399:TYR:HB2	1.99	0.44
2:B:420:LEU:HD11	2:B:459:MET:CE	2.48	0.44
2:B:322:MET:HB3	2:B:322:MET:HE2	1.74	0.44
2:B:434:TYR:CE2	2:B:505:PRO:HB3	2.53	0.44
2:B:533:ILE:HD12	2:B:533:ILE:H	1.82	0.44
1:A:414:ARG:HD3	1:A:460:PRO:O	2.17	0.44
2:B:66:PHE:CD2	2:B:102:GLU:HG3	2.52	0.44
2:B:473:PRO:HB2	2:B:510:PHE:CE1	2.53	0.44
1:A:97:ASN:ND2	1:A:100:GLU:H	2.15	0.43
1:A:241:ARG:NH2	2:B:408:LYS:HG2	2.34	0.43
1:A:431:LEU:HD23	1:A:431:LEU:HA	1.80	0.43
1:A:53:THR:HG23	2:B:447:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG23	1:A:86:HIS:HD2	1.83	0.43
1:A:22:GLU:HG2	1:A:23:SER:H	1.83	0.43
2:B:81:ASP:OD1	2:B:81:ASP:N	2.52	0.43
1:A:10:THR:O	1:A:76:VAL:HA	2.19	0.43
1:A:418:PHE:O	1:A:421:PHE:HB3	2.18	0.43
1:A:265:ILE:HG23	1:A:318:TRP:CE3	2.54	0.43
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.89	0.43
1:A:261:THR:HG23	1:A:313:THR:OG1	2.18	0.43
2:B:195:LYS:HE2	2:B:195:LYS:HB3	1.77	0.43
1:A:195:HIS:C	1:A:196:LEU:HD12	2.43	0.42
1:A:345:ARG:NH1	2:B:529:GLY:O	2.53	0.42
2:B:176:ILE:HG22	2:B:181:GLY:HA2	2.01	0.42
1:A:345:ARG:HB2	1:A:346:PRO:HD3	2.01	0.42
2:B:486:LEU:HD12	2:B:486:LEU:HA	1.78	0.42
2:B:277:ALA:O	2:B:284:GLU:HA	2.19	0.42
2:B:188:ILE:HD13	2:B:196:ASN:HB3	2.02	0.42
1:A:49:LYS:NZ	1:A:57:GLU:OE1	2.45	0.42
1:A:261:THR:HG22	1:A:282:GLU:CB	2.50	0.42
1:A:422:MET:HG2	2:B:256:PHE:CE2	2.55	0.41
2:B:66:PHE:HD2	2:B:102:GLU:HG3	1.85	0.41
2:B:459:MET:HE3	2:B:462:ARG:NH2	2.35	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.87	0.41
1:A:155:GLY:HA2	1:A:200:GLN:OE1	2.20	0.41
1:A:248:ASN:O	1:A:251:VAL:HG12	2.20	0.41
2:B:339:GLN:HE21	2:B:344:LYS:CB	2.27	0.41
1:A:563:LYS:HG3	1:A:564:PRO:HD2	2.02	0.41
1:A:444:PRO:HG2	2:B:368:GLN:HA	2.03	0.41
2:B:91:ALA:O	2:B:95:VAL:HG23	2.21	0.41
2:B:155:MET:HB3	2:B:200:MET:HE3	2.03	0.41
2:B:214:ALA:HB1	2:B:249:THR:O	2.21	0.41
2:B:314:HIS:CD2	2:B:338:SER:HB2	2.56	0.41
1:A:216:SER:OG	1:A:218:VAL:O	2.38	0.40
1:A:513:ILE:CD1	1:A:528:GLN:HG2	2.51	0.40
2:B:504:THR:HG22	2:B:505:PRO:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	527/718 (73%)	504 (96%)	23 (4%)	0	100	100
2	B	487/538 (90%)	463 (95%)	23 (5%)	1 (0%)	43	63
All	All	1014/1256 (81%)	967 (95%)	46 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	494	SER

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	469/648 (72%)	460 (98%)	9 (2%)	50	76
2	B	415/468 (89%)	410 (99%)	5 (1%)	63	83
All	All	884/1116 (79%)	870 (98%)	14 (2%)	55	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	219	SER
1	A	231	THR
1	A	247	LEU
1	A	364	GLN

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Mol	Chain	Res	Type
1	A	402	ILE
1	A	432	ASP
1	A	525	ARG
1	A	531	ILE
2	B	89	GLU
2	B	93	VAL
2	B	302	ILE
2	B	392	GLN
2	B	488	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	97	ASN
1	A	99	GLN
1	A	180	GLN
1	A	192	ASN
1	A	242	HIS
1	A	324	ASN
1	A	493	ASN
2	B	100	GLN
2	B	301	GLN
2	B	333	HIS
2	B	339	GLN
2	B	368	GLN
2	B	402	ASN
2	B	422	ASN
2	B	431	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/718 (74%)	0.37	53 (9%) 13 11	51, 100, 162, 205	0
2	B	495/538 (92%)	0.29	46 (9%) 14 12	49, 84, 159, 214	0
All	All	1030/1256 (82%)	0.33	99 (9%) 13 11	49, 96, 161, 214	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	119	LEU	13.6
2	B	526	ILE	11.3
2	B	537	ALA	10.1
2	B	496	TYR	9.7
1	A	41	ILE	8.8
1	A	33	LEU	8.4
2	B	513	SER	8.1
2	B	528	VAL	7.7
2	B	296	GLU	7.2
2	B	525	ASP	7.2
1	A	116	ASP	7.0
1	A	514	SER	6.7
1	A	523	PRO	6.6
2	B	297	ASN	6.5
1	A	42	ILE	6.3
1	A	274	ASN	6.1
1	A	3	ILE	6.0
1	A	2	LYS	5.7
1	A	150	ASN	5.5
2	B	493	THR	5.4
1	A	515	THR	5.3
1	A	0	PHE	5.2
2	B	281	GLU	5.1
2	B	240	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	494	SER	5.0
1	A	117	PRO	4.9
1	A	152	GLU	4.9
1	A	564	PRO	4.8
2	B	495	GLU	4.7
2	B	142	PHE	4.7
1	A	1	MET	4.3
1	A	516	VAL	4.2
1	A	148	MET	4.2
1	A	273	ALA	4.2
1	A	293	PHE	4.2
2	B	280	LYS	4.1
2	B	88	LEU	4.0
2	B	341	ASP	4.0
1	A	149	GLU	3.9
1	A	114	ARG	3.7
2	B	285	VAL	3.6
1	A	270	GLU	3.6
2	B	469	GLU	3.5
1	A	45	ALA	3.5
1	A	271	GLN	3.5
2	B	342	SER	3.4
1	A	560	CYS	3.4
1	A	118	GLU	3.4
2	B	140	ASN	3.4
1	A	32	MET	3.4
1	A	370	SER	3.2
2	B	141	ARG	3.2
2	B	81	ASP	3.2
1	A	146	LEU	3.2
2	B	429	LYS	3.1
1	A	325	ASN	3.0
2	B	300	ASN	3.0
1	A	323	THR	3.0
1	A	369	GLY	3.0
2	B	417	GLN	3.0
1	A	147	LEU	3.0
2	B	421	ARG	3.0
2	B	511	SER	2.9
2	B	243	ILE	2.9
1	A	292	ASP	2.8
1	A	195	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	298	SER	2.7
1	A	312	GLU	2.7
1	A	524	LYS	2.6
2	B	377	GLU	2.6
2	B	344	LYS	2.6
1	A	275	THR	2.6
1	A	43	PRO	2.5
1	A	526	ASP	2.5
1	A	367	LYS	2.5
2	B	302	ILE	2.5
1	A	154	VAL	2.5
1	A	324	ASN	2.5
1	A	46	PRO	2.4
2	B	507	HIS	2.4
2	B	238	GLU	2.4
2	B	343	LYS	2.4
2	B	118	CYS	2.4
1	A	364	GLN	2.3
1	A	436	LYS	2.2
2	B	382	GLU	2.2
1	A	525	ARG	2.2
1	A	438	ASP	2.2
2	B	491	THR	2.2
1	A	136	ILE	2.2
2	B	512	GLY	2.1
1	A	563	LYS	2.1
2	B	431	GLN	2.1
2	B	239	GLU	2.1
2	B	428	GLU	2.1
1	A	27	HIS	2.1
2	B	527	GLY	2.0
2	B	117	GLY	2.0
1	A	368	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	600	1/1	0.16	0.67	176,176,176,176	0

6.5 Other polymers [i](#)

There are no such residues in this entry.