



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:28 PM BST

PDB ID : 6Y23
Title : DDR1 kinase autoinhibited by its juxtamembrane region
Authors : Sammon, D.; Hohenester, E.; Leitinger, B.
Deposited on : 2020-02-14
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

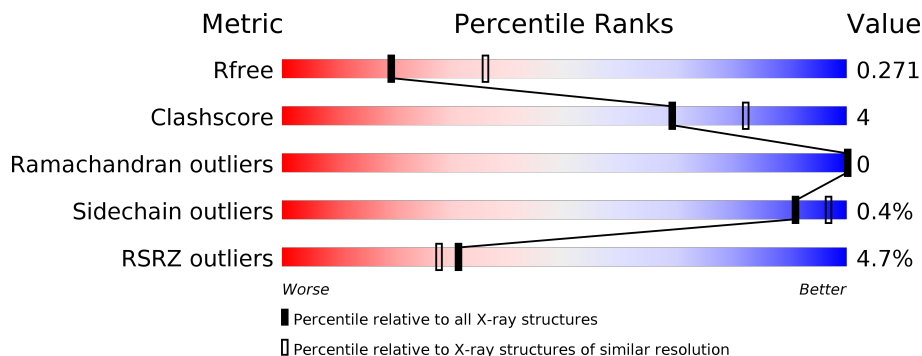
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 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	350	 4% 78% 9% 13%
1	B	350	 2% 81% 5% 14%
1	C	350	 6% 79% 8% 13%

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
2	SO4	A	1001	-	-	X	-
2	SO4	A	1005	-	-	X	-
2	SO4	C	1002	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14337 atoms, of which 7078 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 Epithelial discoidin domain-containing receptor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	305	4723	1525	2336	412	432	18	0	0	0
1	B	301	4737	1523	2356	414	426	18	0	0	0
1	C	305	4797	1539	2386	419	435	18	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	GLY	-	expression tag	UNP Q08345
A	565	PRO	-	expression tag	UNP Q08345
A	569	PHE	TYR	engineered mutation	UNP Q08345
A	586	PHE	TYR	engineered mutation	UNP Q08345
B	564	GLY	-	expression tag	UNP Q08345
B	565	PRO	-	expression tag	UNP Q08345
B	569	PHE	TYR	engineered mutation	UNP Q08345
B	586	PHE	TYR	engineered mutation	UNP Q08345
C	564	GLY	-	expression tag	UNP Q08345
C	565	PRO	-	expression tag	UNP Q08345
C	569	PHE	TYR	engineered mutation	UNP Q08345
C	586	PHE	TYR	engineered mutation	UNP Q08345

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

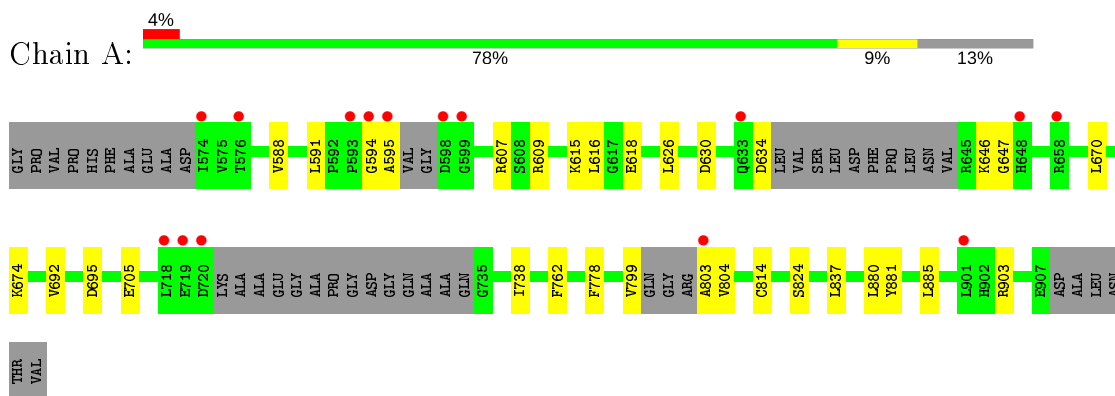
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	15	Total O 15 15	0	0
3	C	8	Total O 8 8	0	0

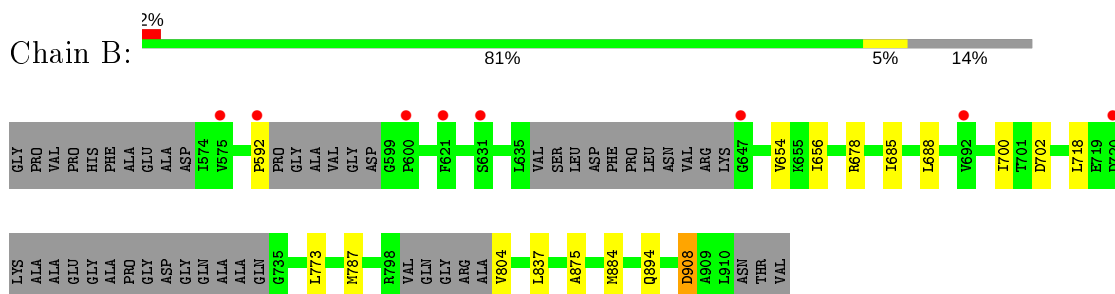
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

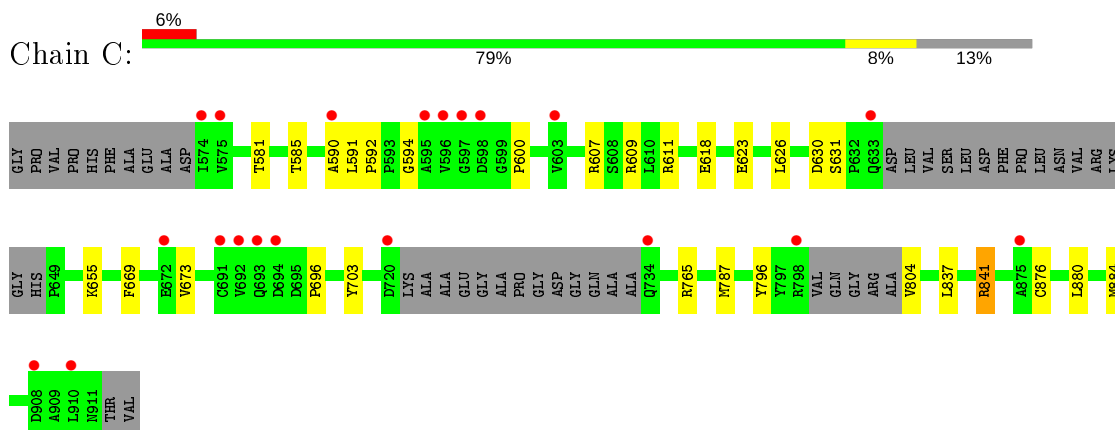
- Molecule 1: Epithelial discoidin domain-containing receptor 1



- Molecule 1: Epithelial discoidin domain-containing receptor 1



- Molecule 1: Epithelial discoidin domain-containing receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.31Å 105.31Å 406.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.42 – 2.58 54.42 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.42-2.58) 99.9 (54.42-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.18rc1_3769, PHENIX 1.18rc1_3769	Depositor
R, R_{free}	0.225 , 0.270 0.226 , 0.271	Depositor DCC
R_{free} test set	2175 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtrriage
Anisotropy	0.313	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14337	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.26	0/2441	0.43	0/3310
1	B	0.26	0/2435	0.45	0/3299
1	C	0.26	0/2466	0.42	0/3342
All	All	0.26	0/7342	0.43	0/9951

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2387	2336	2337	23	0
1	B	2381	2356	2353	11	0
1	C	2411	2386	2385	21	0
2	A	25	0	0	6	0
2	B	5	0	0	0	0
2	C	10	0	0	2	0
3	A	17	0	0	0	0
3	B	15	0	0	1	0
3	C	8	0	0	1	0
All	All	7259	7078	7075	53	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 4.

All (53) 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:609:ARG:NH1	1:A:630:ASP:O	2.08	0.87
1:C:611:ARG:NH1	1:C:630:ASP:OD2	2.09	0.85
1:C:841:ARG:NH1	2:C:1002:SO4:O1	2.12	0.82
1:B:894:GLN:OE1	3:B:1101:HOH:O	2.07	0.71
1:C:585:THR:O	1:C:765:ARG:NH1	2.24	0.70
2:A:1001:SO4:O3	1:C:594:GLY:N	2.25	0.70
1:A:647:GLY:N	2:A:1005:SO4:O4	2.26	0.68
1:A:595:ALA:HB2	1:C:600:PRO:HD2	1.77	0.65
1:B:787:MET:CE	1:B:804:VAL:HG13	2.25	0.65
1:A:594:GLY:N	2:A:1001:SO4:O4	2.31	0.64
1:A:903:ARG:NH1	2:A:1004:SO4:O4	2.31	0.63
1:C:626:LEU:HD21	1:C:703:TYR:CD2	2.35	0.61
1:A:881:TYR:CE2	1:A:885:LEU:HD11	2.36	0.61
1:C:837:LEU:HD12	1:C:884:MET:CE	2.31	0.61
1:A:646:LYS:N	2:A:1005:SO4:O4	2.37	0.58
1:B:592:PRO:O	1:B:678:ARG:NH2	2.38	0.56
1:B:787:MET:HE2	1:B:804:VAL:HG13	1.86	0.56
1:A:616:LEU:HD11	1:A:626:LEU:HD21	1.87	0.56
1:A:705:GLU:N	1:A:705:GLU:OE1	2.39	0.55
1:C:837:LEU:HD12	1:C:884:MET:HE1	1.89	0.54
1:A:670:LEU:HD12	1:C:590:ALA:HB1	1.89	0.54
1:C:796:TYR:HB3	1:C:804:VAL:HG22	1.90	0.54
1:A:588:VAL:HG11	1:A:591:LEU:HD11	1.91	0.53
1:A:799:VAL:N	1:A:803:ALA:O	2.42	0.53
1:B:837:LEU:HD12	1:B:884:MET:CE	2.39	0.53
1:A:674:LYS:NZ	2:A:1001:SO4:O2	2.42	0.51
1:A:607:ARG:NH1	1:A:695:ASP:O	2.43	0.50
1:C:609:ARG:NH1	1:C:631:SER:O	2.44	0.50
1:B:654:VAL:HG12	1:B:656:ILE:HG12	1.95	0.49
1:B:718:LEU:HD22	1:B:875:ALA:HB2	1.94	0.48
1:C:607:ARG:NH2	1:C:696:PRO:O	2.46	0.47
1:A:609:ARG:NH2	1:A:634:ASP:OD2	2.48	0.47
1:C:581:THR:HG21	1:C:655:LYS:HB3	1.97	0.47
1:A:588:VAL:HG13	1:A:762:PHE:CE1	2.50	0.46
1:A:837:LEU:HD11	1:A:880:LEU:HD21	1.97	0.46
1:C:787:MET:HE2	1:C:804:VAL:HG13	1.99	0.45
1:B:700:ILE:HD12	1:B:700:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:VAL:HG11	1:C:592:PRO:HB3	2.00	0.44
1:C:787:MET:CE	1:C:804:VAL:HG13	2.48	0.44
1:C:837:LEU:HD12	1:C:884:MET:HE3	1.99	0.43
1:B:688:LEU:HD11	1:B:702:ASP:HB3	2.00	0.43
1:A:814:CYS:SG	1:A:824:SER:HB2	2.59	0.43
2:C:1002:SO4:O2	3:C:1101:HOH:O	2.16	0.43
1:C:837:LEU:HD11	1:C:880:LEU:HD23	2.01	0.42
1:B:685:ILE:CD1	1:B:773:LEU:HD12	2.49	0.42
1:A:738:ILE:HD12	1:A:778:PHE:CE1	2.55	0.41
1:C:669:PHE:O	1:C:673:VAL:HG23	2.20	0.41
1:C:837:LEU:HD13	1:C:876:CYS:SG	2.60	0.41
1:B:908:ASP:N	1:B:908:ASP:OD1	2.47	0.41
1:C:618:GLU:HA	1:C:623:GLU:HA	2.02	0.41
1:A:616:LEU:HG	1:A:626:LEU:HG	2.03	0.40
1:A:615:LYS:NZ	1:A:618:GLU:OE1	2.42	0.40
1:A:804:VAL:O	1:A:804:VAL:HG13	2.20	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	295/350 (84%)	285 (97%)	10 (3%)	0	100	100
1	B	291/350 (83%)	277 (95%)	14 (5%)	0	100	100
1	C	297/350 (85%)	280 (94%)	17 (6%)	0	100	100
All	All	883/1050 (84%)	842 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	253/292 (87%)	253 (100%)	0	100	100
1	B	255/292 (87%)	254 (100%)	1 (0%)	91	97
1	C	259/292 (89%)	257 (99%)	2 (1%)	81	92
All	All	767/876 (88%)	764 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	908	ASP
1	C	591	LEU
1	C	841	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	1001	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	1005	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	1002	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1001	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.07	0

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.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	SO4	2	0
2	A	1001	SO4	3	0
2	C	1002	SO4	2	0
2	A	1004	SO4	1	0

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	305/350 (87%)	0.58	15 (4%) 29 26	26, 44, 89, 120	0
1	B	301/350 (86%)	0.44	8 (2%) 54 51	26, 39, 76, 103	0
1	C	305/350 (87%)	0.61	20 (6%) 18 15	28, 43, 91, 124	0
All	All	911/1050 (86%)	0.54	43 (4%) 31 28	26, 42, 86, 124	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	595	ALA	7.1
1	A	803	ALA	7.0
1	C	595	ALA	5.1
1	C	734	GLN	4.7
1	A	598	ASP	4.6
1	A	574	ILE	4.4
1	C	597	GLY	4.1
1	B	720	ASP	4.1
1	C	692	VAL	4.0
1	C	720	ASP	3.6
1	C	574	ILE	3.6
1	C	596	VAL	3.4
1	C	910	LEU	3.3
1	C	598	ASP	2.9
1	A	720	ASP	2.9
1	C	633	GLN	2.9
1	C	694	ASP	2.9
1	B	692	VAL	2.9
1	C	575	VAL	2.8
1	A	599	GLY	2.8
1	C	603	VAL	2.8
1	B	647	GLY	2.8
1	B	631	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	593	PRO	2.6
1	C	908	ASP	2.6
1	C	693	GLN	2.6
1	B	600	PRO	2.5
1	A	576	THR	2.5
1	A	648	HIS	2.5
1	B	592	PRO	2.5
1	B	575	VAL	2.4
1	A	658	ARG	2.4
1	C	691	CYS	2.4
1	C	875	ALA	2.3
1	C	672	GLU	2.3
1	C	798	ARG	2.3
1	A	633	GLN	2.2
1	A	594	GLY	2.2
1	A	718	LEU	2.1
1	A	901	LEU	2.1
1	C	590	ALA	2.1
1	B	621	PHE	2.0
1	A	719	GLU	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 monosaccharides 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(\AA^2)	Q<0.9
2	SO4	A	1005	5/5	0.74	0.26	95,97,98,99	0
2	SO4	A	1004	5/5	0.78	0.21	96,97,97,99	0
2	SO4	C	1002	5/5	0.80	0.23	89,93,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	1003	5/5	0.88	0.24	94,94,94,95	0
2	SO4	C	1001	5/5	0.89	0.20	104,104,104,105	0
2	SO4	A	1002	5/5	0.89	0.36	84,86,86,88	0
2	SO4	B	1001	5/5	0.91	0.22	97,98,98,100	0
2	SO4	A	1001	5/5	0.95	0.17	97,98,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.