



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:54 AM UTC

PDB ID : 2V42 / pdb_00002v42
Title : Crystal structure of RseB: a sensor for periplasmic stress response in E. coli
Authors : Wollmann, P.; Zeth, K.
Deposited on : 2007-06-27
Resolution : 2.75 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
Mogul : 2022.3.0, CSD as543be (2022)
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

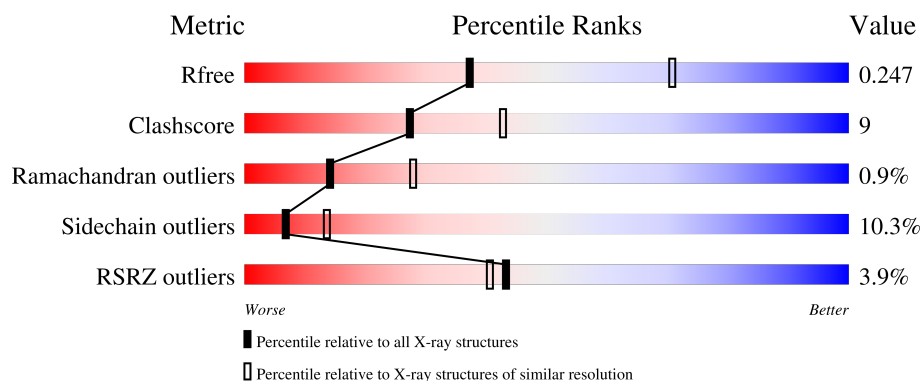
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

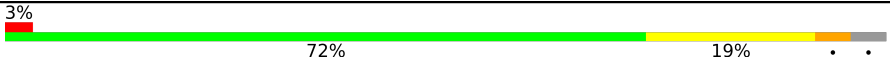
The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	303	
1	B	303	

2 Entry composition [i](#)

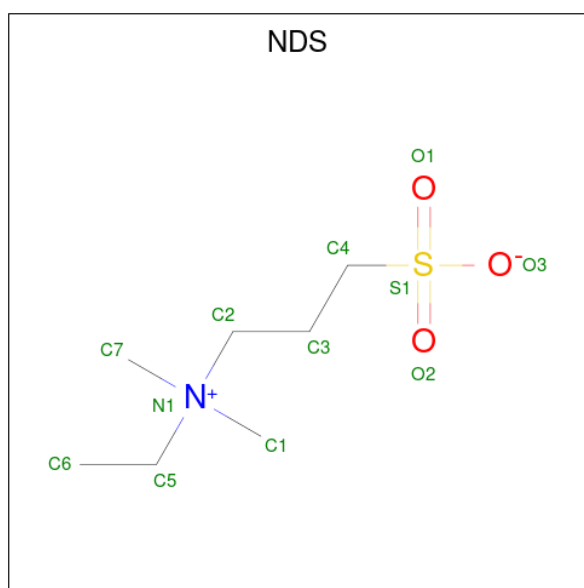
There are 3 unique types of molecules in this entry. The entry contains 4555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIGMA-E FACTOR REGULATORY PROTEIN RSEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2296	1442	404	441	9			
1	B	278	Total	C	N	O	S	0	0	0
			2191	1375	384	423	9			

- Molecule 2 is ETHYL DIMETHYL AMMONIO PROPANE SULFONATE (CCD ID: NDS) (formula: $C_7H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	7	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			12	7	1	3	1		

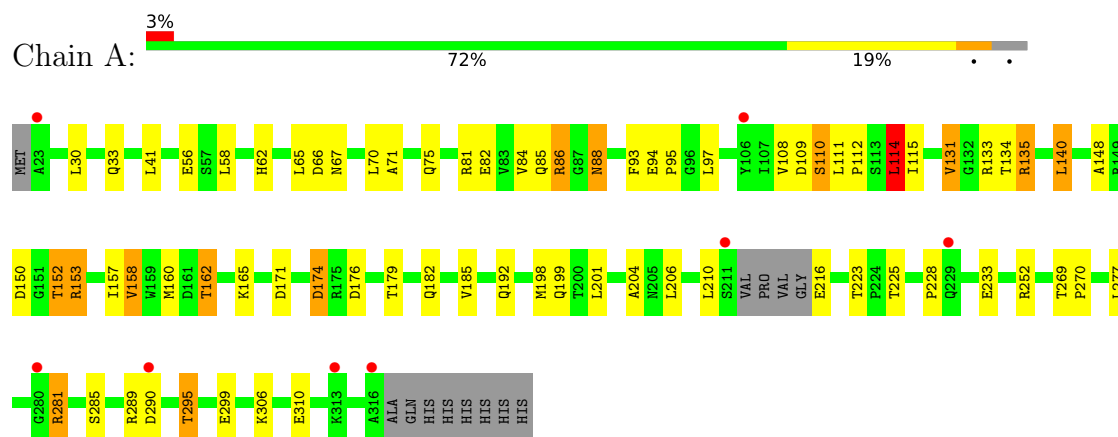
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	19	Total 19	O 19	0	0

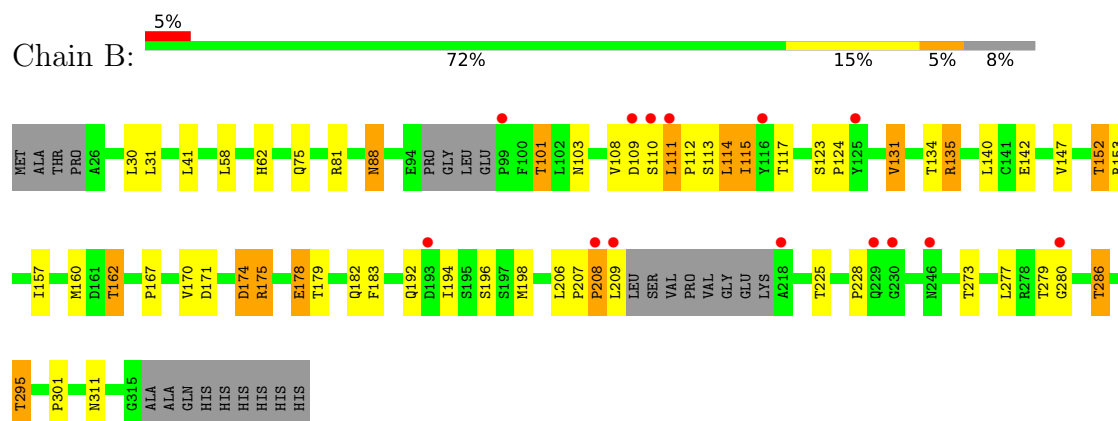
3 Residue-property plots

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: SIGMA-E FACTOR REGULATORY PROTEIN RSEB



• Molecule 1: SIGMA-E FACTOR REGULATORY PROTEIN RSEB



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.29Å 164.29Å 81.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.75) 99.3 (20.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.258 0.209 , 0.247	Depositor DCC
R_{free} test set	1492 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4555	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: NDS

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	0.66	0/2340	0.90	1/3177 (0.0%)
1	B	0.63	1/2233 (0.0%)	0.92	2/3031 (0.1%)
All	All	0.64	1/4573 (0.0%)	0.91	3/6208 (0.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	PRO	CA-C	5.73	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	PRO	N-CA-C	9.99	122.89	110.70
1	A	158	VAL	CB-CA-C	-5.97	101.73	110.81
1	B	108	VAL	N-CA-C	5.03	116.54	108.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	109	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	2296	0	2263	40	0
1	B	2191	0	2130	43	0
2	A	12	0	17	0	0
2	B	12	0	17	1	0
3	A	25	0	0	1	0
3	B	19	0	0	0	0
All	All	4555	0	4427	81	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 9.

All (81) 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:B:152:THR:HG21	1:B:228:PRO:HB3	1.34	1.10
1:A:152:THR:HG22	1:A:153:ARG:HD2	1.38	1.03
1:A:290:ASP:HB2	3:A:2021:HOH:O	1.57	1.02
1:B:152:THR:HG22	1:B:153:ARG:HD2	1.48	0.96
1:B:152:THR:CG2	1:B:153:ARG:HD2	1.97	0.95
1:A:152:THR:HG21	1:A:228:PRO:HB3	1.49	0.91
1:B:206:LEU:C	1:B:208:PRO:HD2	2.05	0.81
1:A:110:SER:OG	1:A:111:LEU:N	2.10	0.80
1:B:114:LEU:HA	1:B:117:THR:OG1	1.87	0.74
1:A:150:ASP:OD1	1:A:152:THR:HB	1.87	0.74
1:B:152:THR:CG2	1:B:228:PRO:HB3	2.18	0.70
1:B:194:ILE:HG22	1:B:198:MET:HB2	1.73	0.69
1:B:112:PRO:HD3	1:B:183:PHE:CE1	2.28	0.69
1:A:233:GLU:OE1	1:A:252:ARG:HD3	1.93	0.69
1:B:206:LEU:O	1:B:208:PRO:HD2	1.94	0.67
1:B:41:LEU:O	1:B:62:HIS:HD2	1.78	0.66
1:A:281:ARG:HB2	1:A:299:GLU:HG3	1.75	0.66
1:A:56:GLU:OE2	1:A:75:GLN:NE2	2.28	0.65
1:B:140:LEU:O	1:B:162:THR:HB	1.99	0.62
1:A:281:ARG:NH1	1:A:299:GLU:OE2	2.34	0.60
1:B:101:THR:HG21	1:B:208:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:CG2	1:B:198:MET:HB2	2.31	0.60
1:B:194:ILE:HD12	1:B:194:ILE:H	1.65	0.60
1:A:140:LEU:O	1:A:162:THR:HB	2.03	0.59
1:B:115:ILE:HG12	1:B:167:PRO:HG3	1.84	0.59
1:B:152:THR:HG23	1:B:153:ARG:HD2	1.83	0.57
1:A:131:VAL:HG22	1:A:131:VAL:O	2.06	0.55
1:B:225:THR:HB	1:B:311:ASN:O	2.08	0.54
1:B:112:PRO:HB2	1:B:114:LEU:HD23	1.87	0.54
1:A:71:ALA:HB3	1:A:85:GLN:HB3	1.90	0.54
1:B:31:LEU:HA	1:B:160:MET:HE1	1.90	0.54
1:A:174:ASP:HB3	1:A:176:ASP:H	1.74	0.52
1:A:201:LEU:C	1:A:201:LEU:HD23	2.34	0.52
1:B:30:LEU:HD13	1:B:142:GLU:HG3	1.91	0.52
1:B:111:LEU:HD12	1:B:112:PRO:HD2	1.93	0.51
1:A:75:GLN:O	1:B:135:ARG:NH2	2.37	0.51
1:A:88:ASN:HD22	1:A:88:ASN:H	1.58	0.50
1:B:112:PRO:HG3	1:B:183:PHE:CD1	2.47	0.49
1:B:279:THR:OG1	1:B:280:GLY:N	2.46	0.49
1:A:131:VAL:O	1:A:131:VAL:CG2	2.60	0.49
1:A:152:THR:CG2	1:A:153:ARG:HD2	2.28	0.49
1:B:171:ASP:OD1	1:B:182:GLN:HG3	2.12	0.49
1:A:114:LEU:HD11	1:A:158:VAL:HG22	1.94	0.48
1:B:175:ARG:HD3	1:B:301:PRO:HG3	1.95	0.48
1:A:269:THR:HB	1:A:270:PRO:HD2	1.96	0.48
1:B:131:VAL:HG22	1:B:131:VAL:O	2.13	0.48
1:A:86:ARG:NH1	1:A:204:ALA:O	2.46	0.48
1:A:33:GLN:NE2	1:A:165:LYS:HE2	2.29	0.48
1:A:70:LEU:HD23	1:A:198:MET:HE3	1.96	0.48
1:B:111:LEU:O	1:B:111:LEU:HG	2.13	0.48
1:B:174:ASP:HB2	1:B:178:GLU:O	2.13	0.48
1:A:114:LEU:HD11	1:A:158:VAL:CG2	2.44	0.47
1:A:171:ASP:CG	1:A:182:GLN:HE21	2.22	0.47
1:B:115:ILE:HD11	1:B:167:PRO:HB3	1.95	0.47
1:A:82:GLU:HB3	1:A:93:PHE:HB2	1.97	0.46
1:B:175:ARG:HB2	2:B:1317:NDS:O2	2.14	0.46
1:A:41:LEU:O	1:A:62:HIS:HD2	1.98	0.45
1:A:135:ARG:NH2	1:B:75:GLN:O	2.37	0.45
1:B:206:LEU:C	1:B:208:PRO:CD	2.84	0.45
1:B:112:PRO:HB2	1:B:114:LEU:CD2	2.46	0.45
1:A:112:PRO:O	1:A:115:ILE:HG12	2.17	0.45
1:A:75:GLN:CD	1:A:81:ARG:HH11	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:O	1:A:109:ASP:HB2	2.17	0.44
1:B:152:THR:HG22	1:B:153:ARG:HH11	1.83	0.44
1:A:30:LEU:C	1:A:160:MET:HE1	2.43	0.44
1:A:33:GLN:HE22	1:A:165:LYS:HE2	1.82	0.44
1:B:75:GLN:HB2	1:B:81:ARG:HB2	1.98	0.44
1:A:148:ALA:CB	1:A:153:ARG:HD3	2.48	0.43
1:A:86:ARG:NH1	1:A:206:LEU:HG	2.34	0.43
1:B:152:THR:HG22	1:B:153:ARG:CD	2.35	0.43
1:B:286:THR:HG23	1:B:295:THR:HB	2.00	0.43
1:B:114:LEU:HD21	1:B:170:VAL:HG11	2.02	0.42
1:A:94:GLU:OE1	1:A:95:PRO:HD2	2.20	0.41
1:B:110:SER:O	1:B:111:LEU:C	2.63	0.41
1:B:123:SER:N	1:B:124:PRO:CD	2.84	0.41
1:A:66:ASP:O	1:A:67:ASN:C	2.64	0.41
1:B:111:LEU:HD12	1:B:112:PRO:CD	2.51	0.41
1:A:84:VAL:HB	1:A:201:LEU:HD11	2.03	0.41
1:A:306:LYS:O	1:A:310:GLU:HG2	2.20	0.41
1:B:88:ASN:O	1:B:103:ASN:HA	2.20	0.41
1:A:285:SER:O	1:A:295:THR:HA	2.22	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	286/303 (94%)	274 (96%)	9 (3%)	3 (1%)	12	24
1	B	272/303 (90%)	255 (94%)	15 (6%)	2 (1%)	18	34
All	All	558/606 (92%)	529 (95%)	24 (4%)	5 (1%)	14	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	PRO
1	A	114	LEU
1	A	174	ASP
1	A	110	SER
1	B	113	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	255/270 (94%)	228 (89%)	27 (11%)	6	13
1	B	241/270 (89%)	217 (90%)	24 (10%)	7	14
All	All	496/540 (92%)	445 (90%)	51 (10%)	7	13

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	65	LEU
1	A	86	ARG
1	A	88	ASN
1	A	97	LEU
1	A	114	LEU
1	A	131	VAL
1	A	133	ARG
1	A	134	THR
1	A	135	ARG
1	A	140	LEU
1	A	152	THR
1	A	153	ARG
1	A	157	ILE
1	A	162	THR
1	A	179	THR
1	A	185	VAL
1	A	192	GLN
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	210	LEU
1	A	216	GLU
1	A	223	THR
1	A	225	THR
1	A	277	LEU
1	A	281	ARG
1	A	289	ARG
1	A	295	THR
1	B	58	LEU
1	B	88	ASN
1	B	101	THR
1	B	111	LEU
1	B	114	LEU
1	B	115	ILE
1	B	131	VAL
1	B	134	THR
1	B	135	ARG
1	B	147	VAL
1	B	152	THR
1	B	157	ILE
1	B	162	THR
1	B	174	ASP
1	B	175	ARG
1	B	178	GLU
1	B	179	THR
1	B	192	GLN
1	B	196	SER
1	B	209	LEU
1	B	273	THR
1	B	277	LEU
1	B	286	THR
1	B	295	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	35	ASN
1	A	39	GLN
1	A	53	GLN
1	A	62	HIS
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	182	GLN
1	A	191	ASN
1	A	205	ASN
1	B	35	ASN
1	B	42	ASN
1	B	62	HIS
1	B	88	ASN
1	B	103	ASN
1	B	182	GLN
1	B	189	ASN
1	B	192	GLN
1	B	264	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NDS	A	1317	-	11,11,11	2.41	1 (9%)	15,16,16	1.47	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDS	B	1317	-	11,11,11	2.62	1 (9%)	15,16,16	1.66	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDS	A	1317	-	-	7/11/11/11	-
2	NDS	B	1317	-	-	9/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1317	NDS	C4-S1	-8.49	1.65	1.77
2	A	1317	NDS	C4-S1	-7.74	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1317	NDS	O1-S1-C4	3.50	112.02	106.73
2	A	1317	NDS	O1-S1-C4	2.98	111.24	106.73
2	A	1317	NDS	O3-S1-C4	2.75	111.39	106.00
2	B	1317	NDS	O2-S1-C4	2.68	110.78	106.73
2	B	1317	NDS	C7-N1-C2	2.45	116.16	109.49
2	A	1317	NDS	C1-N1-C2	2.26	115.64	109.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1317	NDS	N1-C2-C3-C4
2	A	1317	NDS	C3-C2-N1-C5
2	B	1317	NDS	C3-C4-S1-O3
2	A	1317	NDS	C3-C2-N1-C7
2	B	1317	NDS	C3-C2-N1-C1
2	A	1317	NDS	C3-C2-N1-C1
2	B	1317	NDS	C3-C2-N1-C7
2	A	1317	NDS	C3-C4-S1-O3
2	B	1317	NDS	C3-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
2	B	1317	NDS	C6-C5-N1-C7
2	A	1317	NDS	C3-C4-S1-O2
2	B	1317	NDS	C3-C4-S1-O1
2	B	1317	NDS	C3-C4-S1-O2
2	B	1317	NDS	C6-C5-N1-C2
2	A	1317	NDS	C3-C4-S1-O1
2	B	1317	NDS	C6-C5-N1-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1317	NDS	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	290/303 (95%)	0.13	8 (2%) 55 53	32, 65, 85, 93	1 (0%)
1	B	278/303 (91%)	0.26	14 (5%) 34 34	32, 64, 87, 91	1 (0%)
All	All	568/606 (93%)	0.19	22 (3%) 43 40	32, 65, 86, 93	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLN	13.0
1	B	229	GLN	11.1
1	B	209	LEU	5.3
1	B	111	LEU	3.9
1	A	316	ALA	3.5
1	B	109	ASP	3.3
1	A	211	SER	3.1
1	B	218	ALA	2.9
1	A	23	ALA	2.7
1	A	280	GLY	2.5
1	B	280	GLY	2.5
1	A	313	LYS	2.4
1	B	208	PRO	2.4
1	A	106	TYR	2.4
1	B	110	SER	2.3
1	B	193	ASP	2.2
1	A	290	ASP	2.2
1	B	246	ASN	2.1
1	B	116	TYR	2.1
1	B	230	GLY	2.1
1	B	99	PRO	2.0
1	B	125	TYR	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
2	NDS	A	1317	12/12	0.90	0.16	71,76,81,81	0
2	NDS	B	1317	12/12	0.91	0.16	69,77,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.