



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BRQ / pdb_00003brq
Title : Crystal structure of the Escherichia coli transcriptional repressor ascG
Authors : Singer, A.U.; Kagan, O.; Evdokimova, E.; Osipiuk, J.; Joachimiak, A.; Edwards, A.M.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-12-21
Resolution : 2.00 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

<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

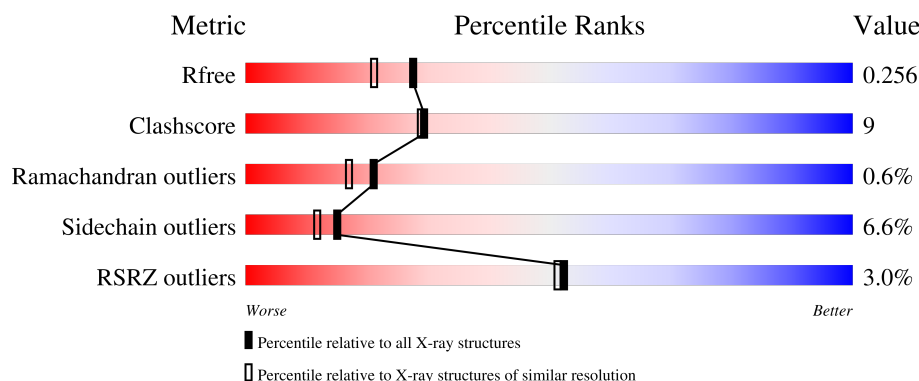
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 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	296	
1	B	296	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4606 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.

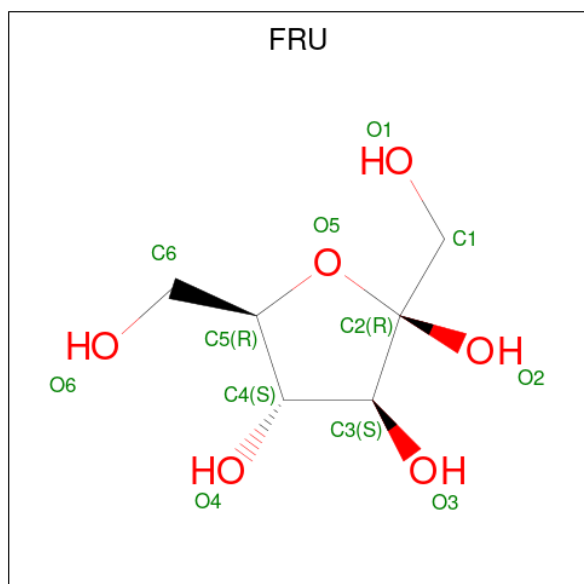
- Molecule 1 is a protein called HTH-type transcriptional regulator ascG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	271	2099	1329	363	396	2	9	0	0	0
1	B	277	2133	1350	369	403	2	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P24242
A	0	HIS	-	expression tag	UNP P24242
B	-1	GLY	-	expression tag	UNP P24242
B	0	HIS	-	expression tag	UNP P24242

- Molecule 2 is beta-D-fructofuranose (CCD ID: FRU) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

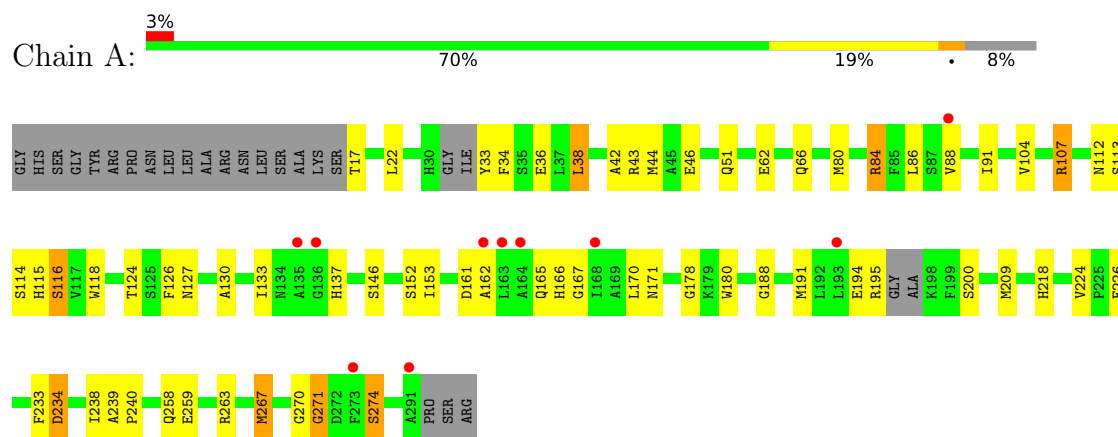
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	220	Total	O	0	0
			220	220		

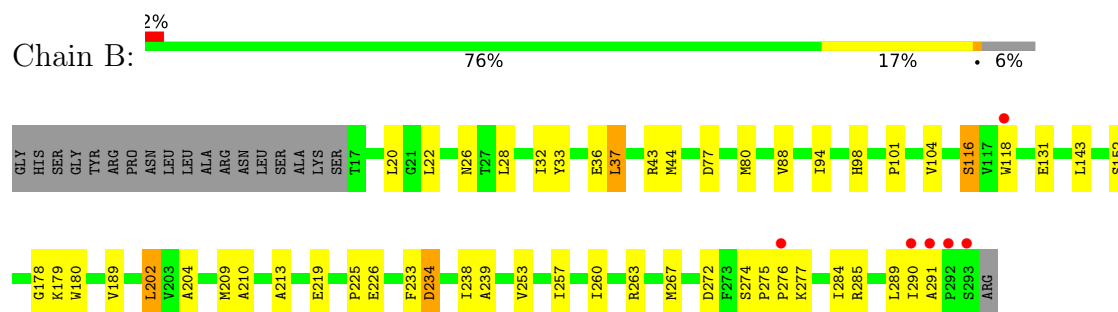
3 Residue-property plots

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: HTH-type transcriptional regulator ascG



- Molecule 1: HTH-type transcriptional regulator ascG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.23Å 65.45Å 130.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 2.00 45.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.08-2.00) 96.9 (45.08-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.22 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.249 0.194 , 0.256	Depositor DCC
R_{free} test set	1760 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4606	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: FRU, NA, 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	0.91	1/2126 (0.0%)	0.99	1/2858 (0.0%)
1	B	1.10	1/2163 (0.0%)	1.09	7/2912 (0.2%)
All	All	1.01	2/4289 (0.0%)	1.04	8/5770 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	213	ALA	CA-CB	5.17	1.61	1.53
1	A	224	VAL	CA-CB	5.08	1.58	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	PRO	O-C-N	6.13	124.13	121.31
1	B	275	PRO	CA-C-N	6.11	127.74	120.23
1	B	275	PRO	C-N-CA	6.11	127.74	120.23
1	B	239	ALA	CA-C-N	-6.01	113.44	120.12
1	B	239	ALA	C-N-CA	-6.01	113.44	120.12
1	B	116	SER	N-CA-C	5.58	118.58	109.59
1	B	226	GLU	N-CA-C	5.16	116.58	111.07
1	A	153	ILE	CB-CA-C	-5.09	105.35	112.02

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	2099	0	2107	46	0
1	B	2133	0	2143	35	0
2	A	12	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	B	1	0	0	0	0
5	A	131	0	0	5	0
5	B	220	0	0	3	0
All	All	4606	0	4262	73	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 (73) 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:28:LEU:HD23	5:B:930:HOH:O	1.60	1.01
1:A:43:ARG:NH1	5:A:918:HOH:O	1.98	0.97
1:B:143:LEU:HD13	1:B:202:LEU:HD11	1.50	0.92
1:A:166:HIS:N	1:A:167:GLY:HA2	1.89	0.87
1:A:33:TYR:N	5:A:914:HOH:O	2.07	0.87
1:A:238:ILE:HD13	1:B:238:ILE:CD1	2.13	0.78
1:A:166:HIS:H	1:A:167:GLY:HA2	1.46	0.77
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.50	0.74
1:A:263:ARG:O	1:A:267:MSE:HE2	1.88	0.73
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.06	0.69
1:A:51:GLN:NE2	5:A:916:HOH:O	2.28	0.66
1:A:91:ILE:HG21	1:A:104:VAL:HG21	1.77	0.66
1:A:238:ILE:CD1	1:B:238:ILE:HD13	2.26	0.66
1:A:238:ILE:CD1	1:B:238:ILE:CD1	2.75	0.64
1:B:219:GLU:HG2	5:B:901:HOH:O	1.99	0.63
1:B:131:GLU:OE1	1:B:285:ARG:NE	2.22	0.61
1:B:263:ARG:HH22	1:B:277:LYS:H	1.48	0.61
1:A:62:GLU:O	1:A:66:GLN:HG3	2.01	0.61
1:A:114:SER:HB2	1:A:274:SER:O	2.03	0.59
1:B:225:PRO:HB2	1:B:290:ILE:HG12	1.83	0.59
1:B:263:ARG:NH2	1:B:277:LYS:H	2.01	0.58
1:A:165:GLN:O	1:A:165:GLN:CG	2.52	0.57
1:A:43:ARG:NH1	1:B:26:ASN:HD22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH1	1:B:26:ASN:ND2	2.54	0.55
1:B:263:ARG:HH22	1:B:276:PRO:HA	1.71	0.55
1:A:178:GLY:HA3	1:A:209:MSE:HE1	1.89	0.54
1:A:107:ARG:O	1:A:116:SER:OG	2.24	0.54
1:A:238:ILE:HD13	1:B:238:ILE:HD11	1.87	0.54
1:A:238:ILE:HD11	1:B:238:ILE:HD13	1.89	0.54
1:B:178:GLY:HA3	1:B:209:MSE:HE1	1.90	0.54
1:A:218:HIS:HD2	5:A:848:HOH:O	1.91	0.53
1:A:188:GLY:HA2	1:A:191:MSE:HE3	1.91	0.53
1:A:130:ALA:HA	1:A:133:ILE:HD12	1.91	0.52
1:A:233:PHE:O	1:A:234:ASP:CB	2.56	0.52
1:B:80:MSE:HG3	1:B:260:ILE:HD13	1.93	0.50
1:A:233:PHE:O	1:A:234:ASP:HB2	2.09	0.50
1:A:171:ASN:OD1	1:A:171:ASN:C	2.56	0.49
1:A:137:HIS:HD2	1:A:200:SER:OG	1.96	0.49
1:A:165:GLN:O	1:A:165:GLN:HG3	2.12	0.49
1:A:270:GLY:O	1:A:271:GLY:O	2.31	0.49
1:B:233:PHE:O	1:B:234:ASP:CB	2.61	0.48
1:B:152:SER:HB2	1:B:180:TRP:CZ2	2.50	0.47
1:A:22:LEU:HD13	1:A:80:MSE:HE2	1.97	0.47
1:A:226:GLU:H	1:A:226:GLU:CD	2.23	0.47
1:B:267:MSE:HE1	1:B:272:ASP:O	2.15	0.47
1:B:104:VAL:CG1	1:B:116:SER:HB3	2.46	0.46
1:A:44:MSE:HE2	1:A:258:GLN:O	2.15	0.46
1:A:162:ALA:O	1:A:166:HIS:HD2	1.99	0.45
1:A:166:HIS:N	1:A:167:GLY:CA	2.72	0.45
1:B:178:GLY:HA3	1:B:209:MSE:CE	2.46	0.45
1:B:32:ILE:O	1:B:33:TYR:C	2.59	0.45
1:B:291:ALA:HB2	5:B:921:HOH:O	2.16	0.45
1:A:34:PHE:CZ	1:A:38:LEU:HD12	2.51	0.45
1:B:143:LEU:HD23	1:B:209:MSE:HE2	1.99	0.45
1:B:77:ASP:O	1:B:101:PRO:HD2	2.17	0.44
1:A:238:ILE:HD13	1:B:238:ILE:HD13	1.88	0.44
1:A:112:ASN:HB3	1:A:115:HIS:CD2	2.53	0.43
1:A:42:ALA:O	1:A:46:GLU:HG3	2.19	0.42
1:B:104:VAL:HG13	1:B:116:SER:HB3	1.99	0.42
1:A:259:GLU:O	1:A:263:ARG:HG2	2.20	0.42
1:B:204:ALA:HB3	1:B:210:ALA:HB2	2.01	0.42
1:A:152:SER:HB2	1:A:180:TRP:CZ2	2.54	0.42
1:B:289:LEU:O	1:B:290:ILE:CG2	2.68	0.42
1:A:126:PHE:HD2	1:A:127:ASN:OD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CD2	1:B:36:GLU:HB2	2.55	0.42
1:B:233:PHE:O	1:B:234:ASP:CG	2.63	0.42
1:A:43:ARG:HG2	5:A:857:HOH:O	2.19	0.41
1:A:84:ARG:HD2	1:A:84:ARG:HA	1.70	0.41
1:B:32:ILE:HG23	1:B:253:VAL:HG22	2.02	0.41
1:B:37:LEU:HA	1:B:257:ILE:HG13	2.03	0.41
1:A:239:ALA:HB3	1:A:240:PRO:HD3	2.03	0.40
1:A:178:GLY:HA3	1:A:209:MSE:CE	2.51	0.40
1:B:94:ILE:O	1:B:98:HIS:HD2	2.04	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	265/296 (90%)	255 (96%)	8 (3%)	2 (1%)	16	11
1	B	275/296 (93%)	263 (96%)	11 (4%)	1 (0%)	30	27
All	All	540/592 (91%)	518 (96%)	19 (4%)	3 (1%)	21	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASP
1	A	271	GLY
1	B	234	ASP

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	225/234 (96%)	207 (92%)	18 (8%)	11	8
1	B	228/234 (97%)	216 (95%)	12 (5%)	20	18
All	All	453/468 (97%)	423 (93%)	30 (7%)	15	12

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	36	GLU
1	A	38	LEU
1	A	84	ARG
1	A	86	LEU
1	A	88	VAL
1	A	107	ARG
1	A	113	SER
1	A	116	SER
1	A	118	TRP
1	A	124	THR
1	A	146	SER
1	A	161	ASP
1	A	170	LEU
1	A	194	GLU
1	A	195	ARG
1	A	267	MSE
1	A	274	SER
1	B	20	LEU
1	B	22	LEU
1	B	37	LEU
1	B	43	ARG
1	B	44	MSE
1	B	88	VAL
1	B	118	TRP
1	B	179	LYS
1	B	189	VAL
1	B	202	LEU
1	B	274	SER
1	B	284	ILE

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

Mol	Chain	Res	Type
1	A	51	GLN
1	A	112	ASN
1	A	115	HIS
1	A	137	HIS
1	A	165	GLN
1	A	166	HIS
1	B	26	ASN
1	B	98	HIS
1	B	106	ASN
1	B	123	GLN
1	B	218	HIS

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	SO4	B	801	-	4,4,4	0.46	0	6,6,6	0.81	0
2	FRU	A	701	-	11,12,12	0.73	0	10,18,18	0.56	0
3	SO4	A	802	-	4,4,4	0.30	0	6,6,6	0.27	0

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	FRU	A	701	-	-	4/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FRU	O1-C1-C2-C3
2	A	701	FRU	O1-C1-C2-O2
2	A	701	FRU	O1-C1-C2-O5
2	A	701	FRU	O5-C5-C6-O6

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	262/296 (88%)	0.42	10 (3%) 44 43	20, 34, 55, 59	0
1	B	268/296 (90%)	-0.04	6 (2%) 62 61	17, 26, 41, 55	0
All	All	530/592 (89%)	0.19	16 (3%) 52 51	17, 29, 50, 59	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	ALA	3.6
1	B	276	PRO	3.3
1	A	164	ALA	3.0
1	A	136	GLY	2.7
1	A	168	ILE	2.7
1	A	273	PHE	2.6
1	A	291	ALA	2.5
1	B	118	TRP	2.4
1	B	290	ILE	2.3
1	B	293	SER	2.3
1	A	88	VAL	2.3
1	A	162	ALA	2.2
1	A	135	ALA	2.1
1	A	163	LEU	2.1
1	A	193	LEU	2.0
1	B	292	PRO	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	FRU	A	701	12/12	0.83	0.14	67,70,72,72	0
3	SO4	A	802	5/5	0.92	0.08	54,54,56,57	0
4	NA	B	601	1/1	0.95	0.08	24,24,24,24	0
3	SO4	B	801	5/5	0.98	0.06	24,25,27,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.