



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 07:13 PM EDT

PDB ID : 3KGL / pdb_00003kgl
Title : Crystal structure of procruciferin, 11S globulin from Brassica napus
Authors : Tandang-Silvas, M.R.; Mikami, B.; Maruyama, N.; Utsumi, S.
Deposited on : 2009-10-29
Resolution : 2.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

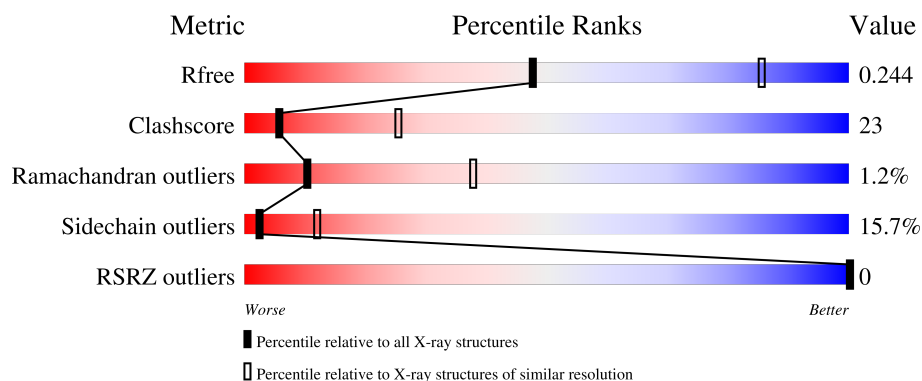
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	466	
1	B	466	
1	C	466	
1	D	466	
1	E	466	

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Mol	Chain	Length	Quality of chain
1	F	466	 A horizontal bar chart showing the quality of chain 1. The bar is divided into four segments: green (43%), yellow (34%), orange (7%), and grey (15%).

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	GOL	D	467	-	-	X	-
2	GOL	E	467	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18711 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 Cruciferin.

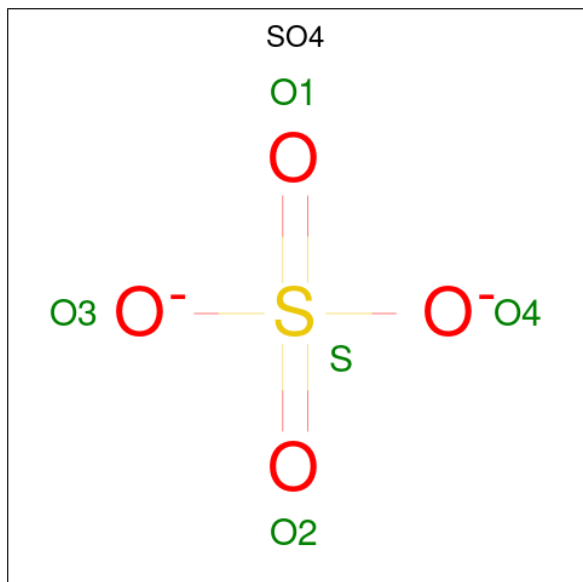
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3134	1969	569	588	8			
1	B	387	Total	C	N	O	S	0	0	0
			3042	1909	554	571	8			
1	C	387	Total	C	N	O	S	0	0	0
			3046	1909	556	573	8			
1	D	390	Total	C	N	O	S	0	0	0
			3067	1923	561	575	8			
1	E	389	Total	C	N	O	S	0	0	0
			3061	1920	558	575	8			
1	F	396	Total	C	N	O	S	0	1	0
			3119	1958	568	585	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

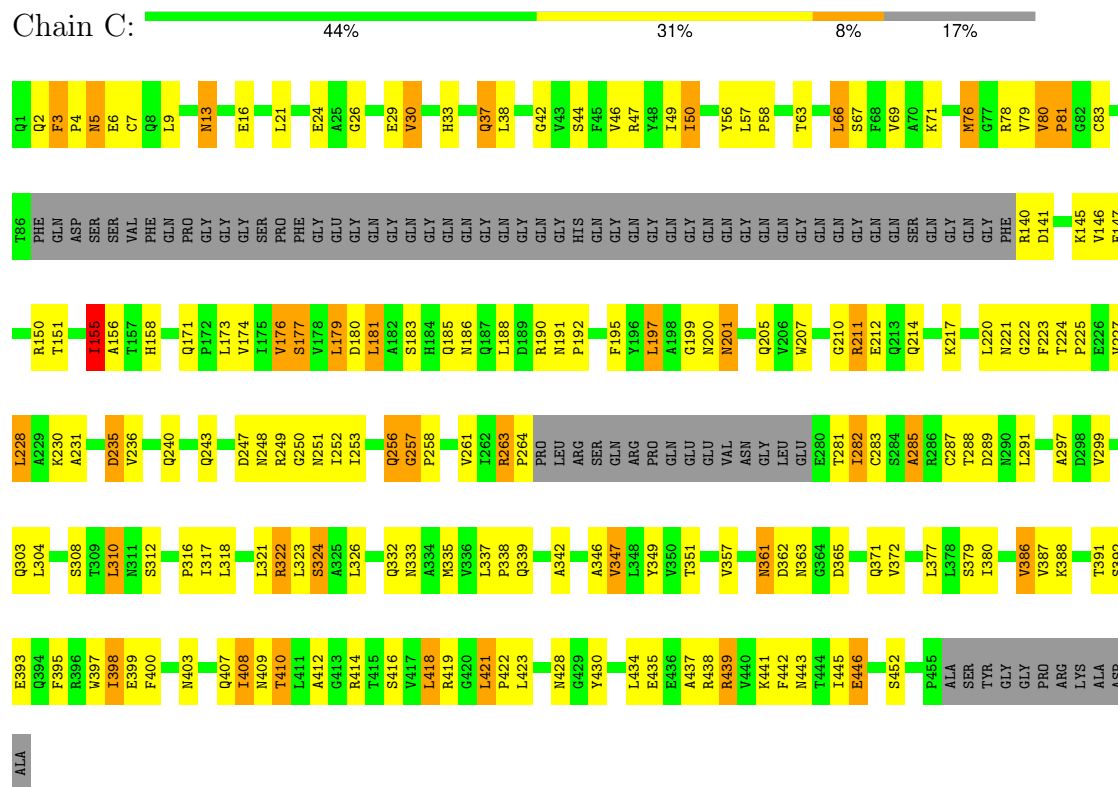
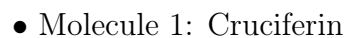
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



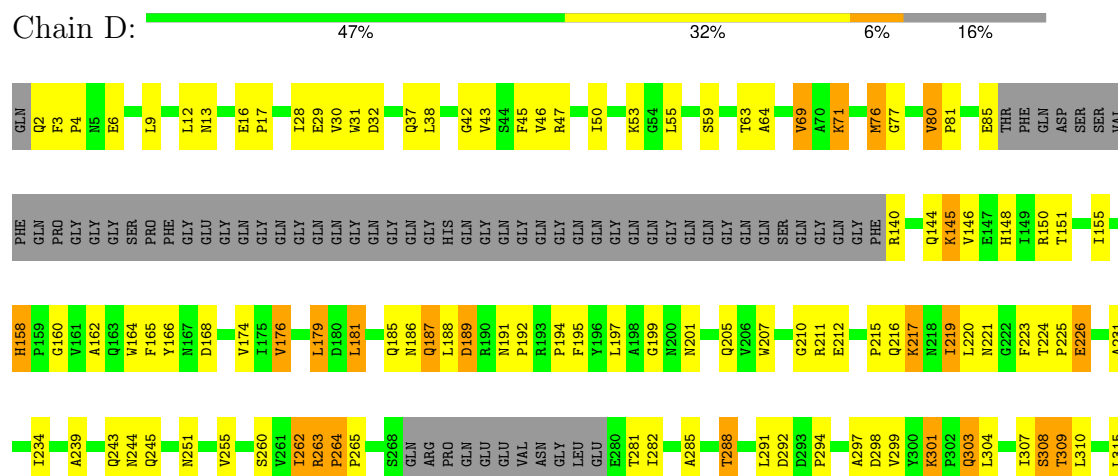
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

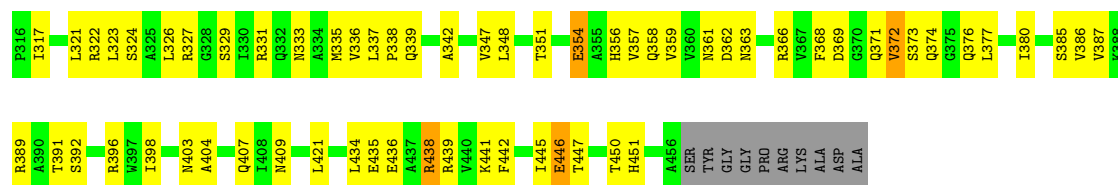
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total 29	O 29	0	0
4	B	37	Total 37	O 37	0	0
4	C	25	Total 25	O 25	0	0
4	D	44	Total 44	O 44	0	0
4	E	27	Total 27	O 27	0	0
4	F	24	Total 24	O 24	0	0

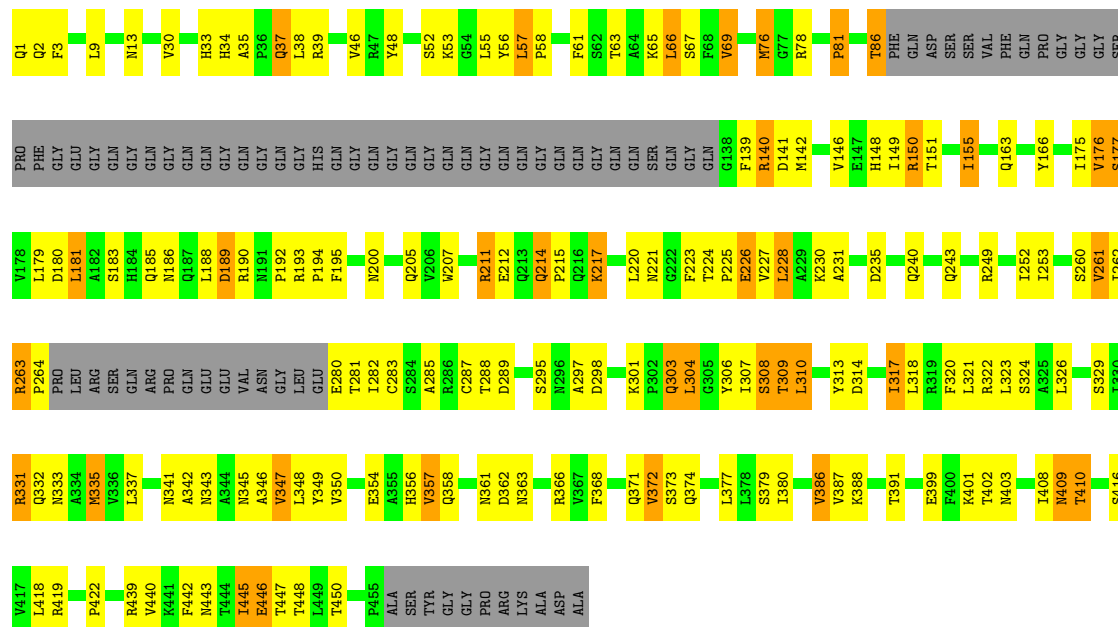


- Molecule 1: Cruciferin

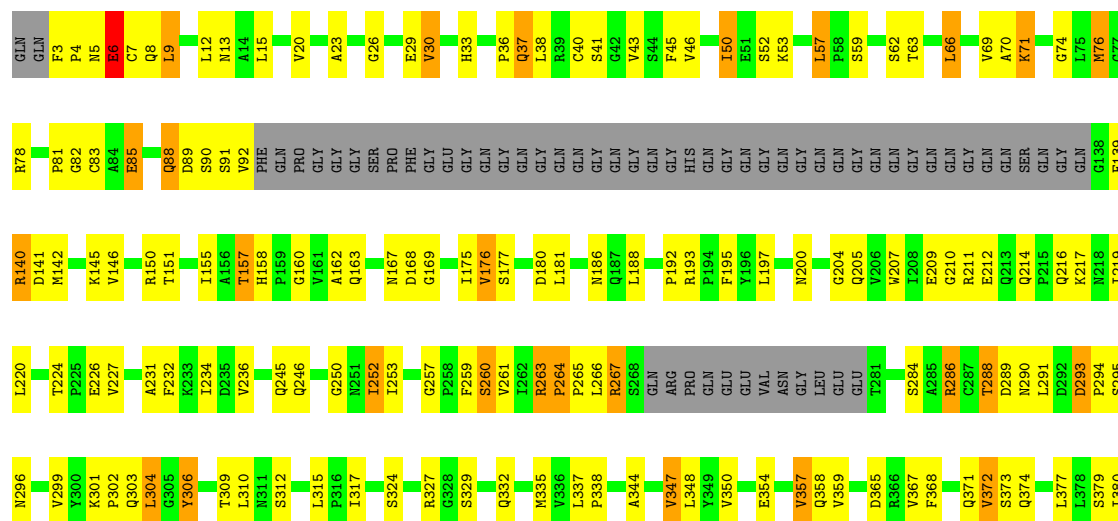


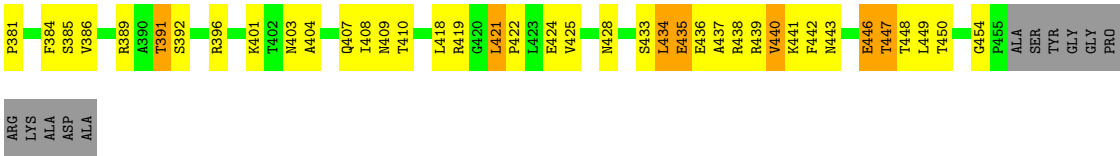


• Molecule 1: Cruciferin



• Molecule 1: Cruciferin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.10Å 190.41Å 99.90Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.98 49.79 – 2.98	Depositor EDS
% Data completeness (in resolution range)	94.4 (49.79-2.98) 94.4 (49.79-2.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.96Å)	Xtriage
Refinement program	CNS, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.158 , 0.250 0.152 , 0.244	Depositor DCC
R_{free} test set	3296 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.459 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18711	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: SO4, GOL

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	0.54	0/3200	0.90	8/4346 (0.2%)
1	B	0.56	0/3105	0.91	10/4218 (0.2%)
1	C	0.54	0/3108	0.96	16/4221 (0.4%)
1	D	0.56	0/3130	0.88	6/4251 (0.1%)
1	E	0.56	0/3124	0.92	4/4242 (0.1%)
1	F	0.52	0/3187	0.92	9/4329 (0.2%)
All	All	0.55	0/18854	0.92	53/25607 (0.2%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	GLU	CA-C-N	-8.06	112.05	120.03
1	D	16	GLU	C-N-CA	-8.06	112.05	120.03
1	C	201	ASN	CA-C-N	7.23	127.07	119.05
1	C	201	ASN	C-N-CA	7.23	127.07	119.05
1	A	293	ASP	CA-C-N	7.13	126.83	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	LEU	Peptide
1	C	188	LEU	Peptide

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	3134	0	3079	180	0
1	B	3042	0	2995	170	0
1	C	3046	0	2998	160	0
1	D	3067	0	3021	138	0
1	E	3061	0	3010	145	0
1	F	3119	0	3069	161	0
2	A	6	0	8	1	0
2	B	6	0	8	1	0
2	C	6	0	8	1	0
2	D	6	0	8	4	0
2	E	6	0	8	4	0
2	F	6	0	8	1	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	F	5	0	0	0	0
4	A	29	0	0	1	0
4	B	37	0	0	1	0
4	C	25	0	0	1	0
4	D	44	0	0	1	0
4	E	27	0	0	0	0
4	F	24	0	0	1	0
All	All	18711	0	18220	852	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 23.

The worst 5 of 852 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:329:SER:OG	1:A:396:ARG:HD2	1.53	1.06
1:D:359:VAL:HG22	1:D:386:VAL:HG22	1.43	1.00
1:C:37:GLN:HG3	1:C:379:SER:HB3	1.45	0.96
1:D:231:ALA:HB2	1:E:335:MET:HE1	1.51	0.93
1:C:361:ASN:HB3	1:C:363:ASN:H	1.34	0.93

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	392/466 (84%)	353 (90%)	33 (8%)	6 (2%)	8	33
1	B	381/466 (82%)	350 (92%)	29 (8%)	2 (0%)	24	58
1	C	381/466 (82%)	350 (92%)	25 (7%)	6 (2%)	7	31
1	D	384/466 (82%)	354 (92%)	28 (7%)	2 (0%)	24	58
1	E	383/466 (82%)	339 (88%)	39 (10%)	5 (1%)	9	36
1	F	391/466 (84%)	349 (89%)	36 (9%)	6 (2%)	8	33
All	All	2312/2796 (83%)	2095 (91%)	190 (8%)	27 (1%)	10	38

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	C	333	ASN
1	A	92	VAL
1	A	244	ASN
1	B	6	GLU

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	343/388 (88%)	286 (83%)	57 (17%)	2	11
1	B	333/388 (86%)	272 (82%)	61 (18%)	2	8
1	C	333/388 (86%)	286 (86%)	47 (14%)	3	15
1	D	335/388 (86%)	285 (85%)	50 (15%)	3	13
1	E	334/388 (86%)	284 (85%)	50 (15%)	3	13
1	F	342/388 (88%)	291 (85%)	51 (15%)	3	13
All	All	2020/2328 (87%)	1704 (84%)	316 (16%)	2	12

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	211	ARG
1	F	220	LEU
1	E	260	SER
1	E	410	THR
1	F	317	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	256	GLN
1	F	144	GLN
1	D	187	GLN
1	F	88	GLN
1	F	296	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	GOL	B	467	-	5,5,5	0.40	0	5,5,5	0.92	0
2	GOL	D	467	-	5,5,5	0.33	0	5,5,5	1.23	1 (20%)
3	SO4	D	473	-	4,4,4	0.24	0	6,6,6	0.21	0
3	SO4	A	474	-	4,4,4	0.26	0	6,6,6	0.10	0
3	SO4	C	472	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	F	475	-	4,4,4	0.25	0	6,6,6	0.16	0
2	GOL	F	467	-	5,5,5	0.44	0	5,5,5	0.35	0
2	GOL	A	467	-	5,5,5	0.30	0	5,5,5	0.71	0
2	GOL	E	467	-	5,5,5	0.30	0	5,5,5	0.98	0
2	GOL	C	467	-	5,5,5	0.38	0	5,5,5	0.87	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	GOL	B	467	-	-	4/4/4/4	-
2	GOL	D	467	-	-	4/4/4/4	-
2	GOL	F	467	-	-	3/4/4/4	-
2	GOL	A	467	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	467	-	-	2/4/4/4	-
2	GOL	C	467	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	467	GOL	O1-C1-C2	-2.01	101.34	110.38

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	467	GOL	C1-C2-C3-O3
2	C	467	GOL	O1-C1-C2-C3
2	D	467	GOL	O1-C1-C2-C3
2	E	467	GOL	C1-C2-C3-O3
2	F	467	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	467	GOL	1	0
2	D	467	GOL	4	0
3	D	473	SO4	1	0
3	A	474	SO4	1	0
2	F	467	GOL	1	0
2	A	467	GOL	1	0
2	E	467	GOL	4	0
2	C	467	GOL	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 [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	398/466 (85%)	-1.61	0 100 100	22, 44, 114, 161	0
1	B	387/466 (83%)	-1.65	0 100 100	18, 41, 99, 161	0
1	C	387/466 (83%)	-1.62	0 100 100	20, 44, 101, 130	0
1	D	390/466 (83%)	-1.63	0 100 100	20, 42, 105, 143	0
1	E	389/466 (83%)	-1.65	0 100 100	22, 45, 99, 154	0
1	F	396/466 (84%)	-1.61	0 100 100	20, 45, 111, 160	1 (0%)
All	All	2347/2796 (83%)	-1.63	0 100 100	18, 43, 105, 161	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	SO4	A	474	5/5	0.98	0.06	54,129,166,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	E	467	6/6	0.99	0.04	18,28,35,40	0
3	SO4	C	472	5/5	0.99	0.04	59,87,126,187	0
3	SO4	D	473	5/5	0.99	0.06	49,84,97,194	0
3	SO4	F	475	5/5	0.99	0.10	66,92,136,148	0
2	GOL	F	467	6/6	1.00	0.03	11,28,49,50	0
2	GOL	B	467	6/6	1.00	0.03	16,29,38,49	0
2	GOL	C	467	6/6	1.00	0.04	17,32,33,41	0
2	GOL	D	467	6/6	1.00	0.03	23,28,34,72	0
2	GOL	A	467	6/6	1.00	0.04	16,20,31,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.