



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 8D30 / pdb_00008d30
Title : Crystal structure of the human COPB2 WD-domains
Authors : Zeng, H.; Dong, A.; Hutchinson, A.; Seitova, A.; Loppnau, P.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on : 2022-05-31
Resolution : 2.40 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

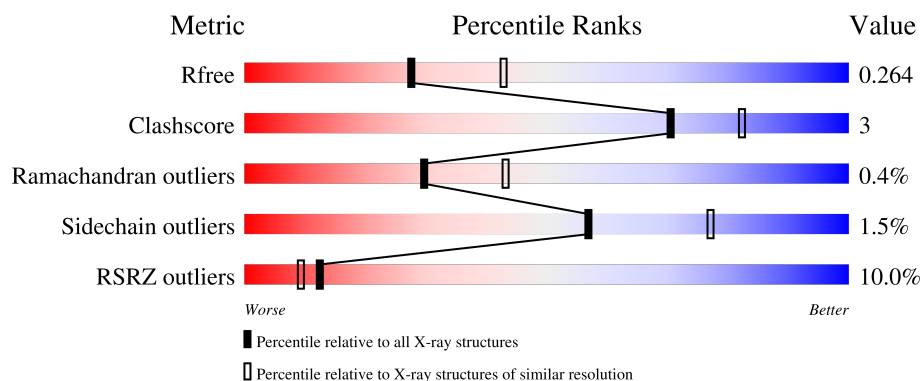
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	615	
1	B	615	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8563 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 Coatomer subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4487	2880	757	826	24			
1	B	550	Total	C	N	O	S	0	1	0
			3992	2547	685	738	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P35606
A	-16	HIS	-	expression tag	UNP P35606
A	-15	HIS	-	expression tag	UNP P35606
A	-14	HIS	-	expression tag	UNP P35606
A	-13	HIS	-	expression tag	UNP P35606
A	-12	HIS	-	expression tag	UNP P35606
A	-11	HIS	-	expression tag	UNP P35606
A	-10	SER	-	expression tag	UNP P35606
A	-9	SER	-	expression tag	UNP P35606
A	-8	GLY	-	expression tag	UNP P35606
A	-7	ARG	-	expression tag	UNP P35606
A	-6	GLU	-	expression tag	UNP P35606
A	-5	ASN	-	expression tag	UNP P35606
A	-4	LEU	-	expression tag	UNP P35606
A	-3	TYR	-	expression tag	UNP P35606
A	-2	PHE	-	expression tag	UNP P35606
A	-1	GLN	-	expression tag	UNP P35606
A	0	GLY	-	expression tag	UNP P35606
B	-17	MET	-	initiating methionine	UNP P35606
B	-16	HIS	-	expression tag	UNP P35606
B	-15	HIS	-	expression tag	UNP P35606
B	-14	HIS	-	expression tag	UNP P35606
B	-13	HIS	-	expression tag	UNP P35606
B	-12	HIS	-	expression tag	UNP P35606
B	-11	HIS	-	expression tag	UNP P35606

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	SER	-	expression tag	UNP P35606
B	-9	SER	-	expression tag	UNP P35606
B	-8	GLY	-	expression tag	UNP P35606
B	-7	ARG	-	expression tag	UNP P35606
B	-6	GLU	-	expression tag	UNP P35606
B	-5	ASN	-	expression tag	UNP P35606
B	-4	LEU	-	expression tag	UNP P35606
B	-3	TYR	-	expression tag	UNP P35606
B	-2	PHE	-	expression tag	UNP P35606
B	-1	GLN	-	expression tag	UNP P35606
B	0	GLY	-	expression tag	UNP P35606

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

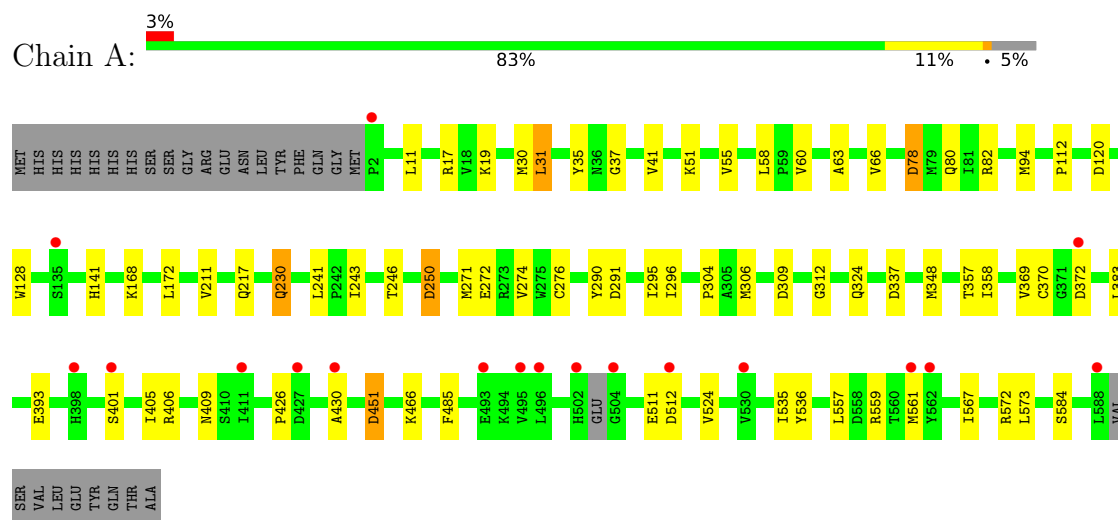
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	32	Total	O	0	0
			32	32		

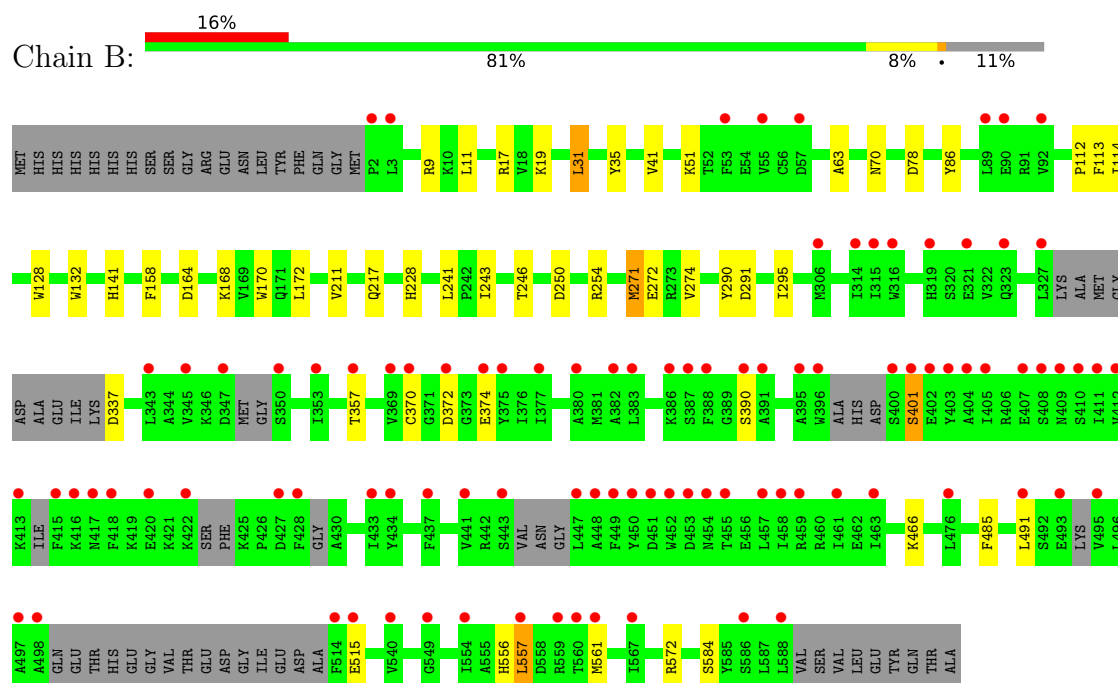
3 Residue-property plots [i](#)

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: Coatomer subunit beta'



• Molecule 1: Coatomer subunit beta'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.07Å 134.06Å 144.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.40 49.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.12-2.40) 99.0 (49.12-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.219 , 0.247 0.231 , 0.264	Depositor DCC
R_{free} test set	2516 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.6	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	0.93	EDS
Total number of atoms	8563	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: EDO

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	0.88	0/4600	1.21	14/6269 (0.2%)
1	B	0.83	0/4084	1.21	13/5578 (0.2%)
All	All	0.86	0/8684	1.21	27/11847 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	LYS	N-CA-C	-7.74	103.44	113.12
1	A	451	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	113	PHE	CA-CB-CG	6.87	120.67	113.80
1	B	466	LYS	N-CA-C	-6.71	104.73	113.12
1	B	164	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	401	SER	CA-C-N	6.42	133.79	121.54
1	B	401	SER	C-N-CA	6.42	133.79	121.54
1	A	120	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	309	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	250	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	485	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	485	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	172	LEU	N-CA-C	5.65	119.27	112.38
1	B	172	LEU	N-CA-C	-5.56	101.62	109.96
1	A	426	PRO	CA-C-N	5.46	127.87	120.38
1	A	426	PRO	C-N-CA	5.46	127.87	120.38
1	B	78	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	66	VAL	N-CA-CB	5.40	118.72	112.40
1	B	557	LEU	CA-C-N	5.33	127.95	120.28
1	B	557	LEU	C-N-CA	5.33	127.95	120.28
1	B	250	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	556	HIS	N-CA-C	-5.30	100.09	108.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	512	ASP	CA-C-N	5.09	127.10	120.28
1	A	512	ASP	C-N-CA	5.09	127.10	120.28
1	A	78	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	337	ASP	CA-CB-CG	5.02	117.62	112.60

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	4487	0	4173	32	0
1	B	3992	0	3467	22	0
2	A	4	0	6	1	0
3	A	48	0	0	0	0
3	B	32	0	0	0	0
All	All	8563	0	7646	54	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 3.

All (54) 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:271:MET:HE2	1:B:295:ILE:HG12	1.62	0.82
1:B:9:ARG:HD2	1:B:295:ILE:HD12	1.77	0.67
1:A:559:ARG:HG2	1:A:561:MET:HE2	1.79	0.64
1:A:535:ILE:HG21	1:A:573:LEU:HD21	1.82	0.60
1:A:358:ILE:HG12	1:A:369:VAL:HG22	1.82	0.59
1:B:114:ILE:HG12	1:B:132:TRP:HZ3	1.66	0.58
1:B:274:VAL:HG22	1:B:290:TYR:CE1	2.41	0.56
1:B:572:ARG:HG2	1:B:584:SER:HB2	1.87	0.55
1:B:31:LEU:HD21	1:B:63:ALA:HB3	1.89	0.55
1:A:31:LEU:HD21	1:A:63:ALA:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HG3	1:A:291:ASP:HA	1.91	0.52
1:A:276:CYS:HB3	2:A:601:EDO:H22	1.92	0.52
1:A:41:VAL:HB	1:A:51:LYS:HB2	1.92	0.52
1:A:271:MET:HB2	1:A:290:TYR:CD2	2.44	0.52
1:A:141:HIS:CE1	1:A:168:LYS:HD2	2.45	0.51
1:B:17:ARG:HG3	1:B:291:ASP:HA	1.92	0.51
1:A:230:GLN:HG2	1:A:250:ASP:HB3	1.91	0.51
1:B:141:HIS:CE1	1:B:168:LYS:HD2	2.46	0.51
1:A:324:GLN:HB2	1:A:348:MET:SD	2.51	0.50
1:B:41:VAL:HB	1:B:51:LYS:HB2	1.94	0.50
1:B:158:PHE:CE2	1:B:170:TRP:HB2	2.48	0.49
1:A:58:LEU:HD12	1:A:78:ASP:HB3	1.96	0.48
1:A:274:VAL:HG22	1:A:290:TYR:CE2	2.49	0.48
1:A:557:LEU:HD13	1:A:561:MET:HB2	1.96	0.47
1:A:409:ASN:HA	1:A:430:ALA:O	2.15	0.47
1:A:272:GLU:HB2	1:A:291:ASP:HB2	1.97	0.47
1:A:19:LYS:HA	1:A:19:LYS:HE2	1.97	0.46
1:A:312:GLY:HA3	1:A:567:ILE:HD11	1.99	0.45
1:A:37:GLY:HA2	1:A:60:VAL:HG23	2.00	0.44
1:A:524:VAL:HG13	1:A:536:TYR:HB2	1.99	0.44
1:B:17:ARG:HB3	1:B:35:TYR:HB2	1.98	0.44
1:A:304:PRO:HG2	1:A:306:MET:HE2	1.99	0.44
1:B:31:LEU:C	1:B:31:LEU:HD23	2.42	0.44
1:B:557:LEU:HD13	1:B:561:MET:HB2	1.99	0.44
1:A:55:VAL:HG13	1:A:82:ARG:HD2	1.98	0.44
1:B:374:GLU:HA	1:B:390:SER:HA	1.99	0.44
1:A:17:ARG:HB3	1:A:35:TYR:HB2	2.00	0.43
1:B:19:LYS:HA	1:B:19:LYS:HE2	1.99	0.43
1:B:211:VAL:HG21	1:B:246:THR:HG21	2.00	0.43
1:B:112:PRO:HA	1:B:128:TRP:CZ2	2.53	0.43
1:B:228:HIS:CE1	1:B:254[A]:ARG:HG3	2.54	0.43
1:B:357:THR:OG1	1:B:370:CYS:HB2	2.19	0.43
1:A:572:ARG:HG2	1:A:584:SER:HB2	2.00	0.43
1:A:112:PRO:HA	1:A:128:TRP:CZ2	2.54	0.42
1:B:491:LEU:HD11	1:B:515:GLU:HG2	2.00	0.42
1:A:357:THR:OG1	1:A:370:CYS:HB2	2.20	0.42
1:A:80:GLN:HG3	1:A:94:MET:HE3	2.02	0.42
1:A:211:VAL:HG21	1:A:246:THR:HG21	2.01	0.42
1:B:241:LEU:HB3	1:B:243:ILE:HG12	2.03	0.41
1:A:241:LEU:HB3	1:A:243:ILE:HG12	2.02	0.41
1:A:348:MET:HE2	1:A:383:LEU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:MET:HB2	1:A:296:ILE:HD11	2.03	0.40
1:A:393:GLU:HB2	1:A:406:ARG:HE	1.87	0.40
1:B:70:ASN:HA	1:B:86:TYR:CZ	2.56	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	583/615 (95%)	553 (95%)	27 (5%)	3 (0%)	24	37
1	B	531/615 (86%)	501 (94%)	28 (5%)	2 (0%)	30	43
All	All	1114/1230 (91%)	1054 (95%)	55 (5%)	5 (0%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	SER
1	A	511	GLU
1	B	272	GLU
1	A	372	ASP
1	B	372	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	444/537 (83%)	437 (98%)	7 (2%)	55	76
1	B	354/537 (66%)	349 (99%)	5 (1%)	59	79
All	All	798/1074 (74%)	786 (98%)	12 (2%)	57	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	31	LEU
1	A	217	GLN
1	A	230	GLN
1	A	295	ILE
1	A	405	ILE
1	A	451	ASP
1	B	11	LEU
1	B	31	LEU
1	B	217	GLN
1	B	271	MET
1	B	401	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	87	ASN
1	A	155	ASN
1	A	223	GLN
1	A	326	ASN
1	A	359	GLN
1	A	398	HIS
1	B	80	GLN
1	B	87	ASN
1	B	111	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	EDO	A	601	-	3,3,3	0.80	0	2,2,2	0.08	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	EDO	A	601	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	EDO	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	586/615 (95%)	0.35	18 (3%)	51	47	18, 52, 79, 140	1 (0%)
1	B	550/615 (89%)	0.92	96 (17%)	4	3	25, 66, 134, 160	1 (0%)
All	All	1136/1230 (92%)	0.62	114 (10%)	12	9	18, 58, 111, 160	2 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	498	ALA	4.8
1	B	443	SER	4.8
1	B	453	ASP	4.4
1	B	428	PHE	4.3
1	B	347	ASP	4.3
1	B	418	PHE	4.3
1	B	452	TRP	4.1
1	A	588	LEU	3.9
1	B	497	ALA	3.8
1	B	380	ALA	3.7
1	B	327	LEU	3.7
1	B	588	LEU	3.7
1	B	463	ILE	3.6
1	B	321	GLU	3.6
1	B	383	LEU	3.6
1	B	455	THR	3.5
1	A	2	PRO	3.4
1	B	495	VAL	3.3
1	B	454	ASN	3.2
1	B	375	TYR	3.2
1	B	415	PHE	3.2
1	A	502	HIS	3.2
1	B	416	LYS	3.2
1	B	515	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	403	TYR	3.1
1	B	401	SER	3.1
1	B	410	SER	3.1
1	B	461	ILE	3.1
1	B	92	VAL	3.1
1	B	458	ILE	3.1
1	B	314	ILE	3.0
1	B	386	LYS	3.0
1	B	450	TYR	2.9
1	B	417	ASN	2.9
1	B	407	GLU	2.9
1	B	459	ARG	2.9
1	B	427	ASP	2.9
1	B	493	GLU	2.9
1	B	405	ILE	2.9
1	B	412	VAL	2.9
1	B	395	ALA	2.8
1	B	404	ALA	2.8
1	B	411	ILE	2.8
1	B	559	ARG	2.8
1	B	350	SER	2.7
1	B	437	PHE	2.7
1	A	411	ILE	2.7
1	A	504	GLY	2.7
1	B	549	GLY	2.7
1	B	400	SER	2.7
1	B	540	VAL	2.7
1	B	449	PHE	2.7
1	B	357	THR	2.7
1	B	3	LEU	2.6
1	B	447	LEU	2.6
1	B	353	ILE	2.6
1	B	554	ILE	2.6
1	B	55	VAL	2.6
1	B	422	LYS	2.6
1	A	427	ASP	2.5
1	B	370	CYS	2.5
1	B	413	LYS	2.5
1	B	396	TRP	2.5
1	B	390	SER	2.5
1	B	402	GLU	2.5
1	A	496	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	562	TYR	2.5
1	B	372	ASP	2.5
1	A	135	SER	2.5
1	B	2	PRO	2.4
1	B	451	ASP	2.4
1	B	90	GLU	2.4
1	B	434	TYR	2.4
1	B	388	PHE	2.4
1	B	560	THR	2.4
1	B	377	ILE	2.4
1	B	319	HIS	2.3
1	B	491	LEU	2.3
1	B	315	ILE	2.3
1	B	316	TRP	2.3
1	B	457	LEU	2.3
1	A	495	VAL	2.3
1	B	345	VAL	2.3
1	B	369	VAL	2.3
1	B	420	GLU	2.2
1	B	323	GLN	2.2
1	B	374	GLU	2.2
1	A	430	ALA	2.2
1	B	306	MET	2.2
1	B	343	LEU	2.2
1	B	567	ILE	2.2
1	B	57	ASP	2.2
1	A	530	VAL	2.1
1	A	561	MET	2.1
1	B	382	ALA	2.1
1	A	372	ASP	2.1
1	A	512	ASP	2.1
1	A	401	SER	2.1
1	B	586	SER	2.1
1	B	514	PHE	2.1
1	B	561	MET	2.1
1	B	448	ALA	2.1
1	B	409	ASN	2.1
1	B	433	ILE	2.1
1	B	387	SER	2.1
1	A	398	HIS	2.1
1	B	53	PHE	2.0
1	B	391	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	441	VAL	2.0
1	A	493	GLU	2.0
1	B	89	LEU	2.0
1	B	476	LEU	2.0
1	B	557	LEU	2.0
1	B	408	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
2	EDO	A	601	4/4	0.87	0.15	52,57,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.