



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:28 AM UTC

PDB ID : 5DOT / pdb_00005dot
Title : Crystal Structure of Human Carbamoyl phosphate synthetase I (CPS1), apo form
Authors : Polo, L.M.; de Cima, S.; Fita, I.; Rubio, V.
Deposited on : 2015-09-11
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

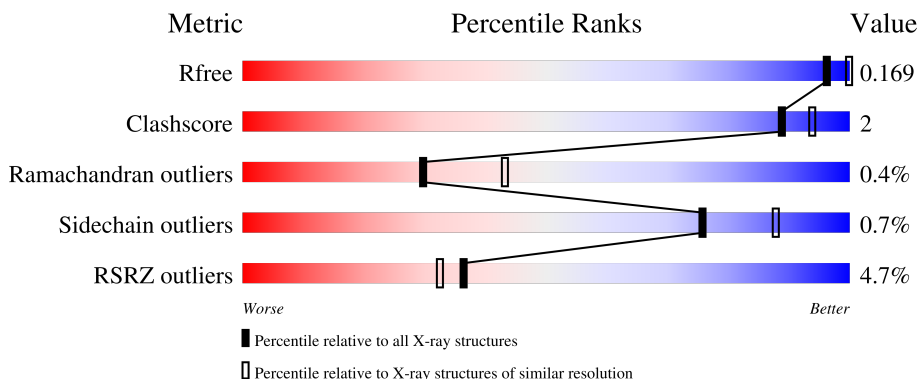
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

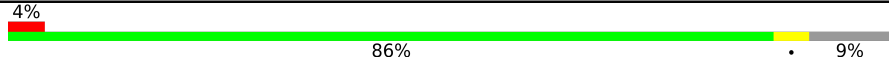
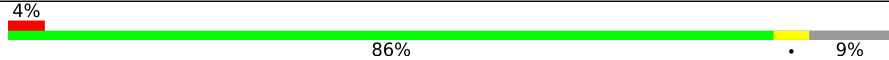
The reported resolution of this entry is 2.40 Å.

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	1489	 4% 86% 9%
1	B	1489	 4% 86% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21866 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 Carbamoyl-phosphate synthase [ammonia], mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1352	10503	6678	1777	1994	54	0	4	0
1	B	1351	10498	6677	1774	1993	54	0	5	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P31327
A	13	SER	-	expression tag	UNP P31327
A	14	TYR	-	expression tag	UNP P31327
A	15	TYR	-	expression tag	UNP P31327
A	16	HIS	-	expression tag	UNP P31327
A	17	HIS	-	expression tag	UNP P31327
A	18	HIS	-	expression tag	UNP P31327
A	19	HIS	-	expression tag	UNP P31327
A	20	HIS	-	expression tag	UNP P31327
A	21	HIS	-	expression tag	UNP P31327
A	22	ASP	-	expression tag	UNP P31327
A	23	TYR	-	expression tag	UNP P31327
A	24	ASP	-	expression tag	UNP P31327
A	25	ILE	-	expression tag	UNP P31327
A	26	PRO	-	expression tag	UNP P31327
A	27	THR	-	expression tag	UNP P31327
A	28	THR	-	expression tag	UNP P31327
A	29	GLU	-	expression tag	UNP P31327
A	30	ASN	-	expression tag	UNP P31327
A	31	LEU	-	expression tag	UNP P31327
A	32	TYR	-	expression tag	UNP P31327
A	33	PHE	-	expression tag	UNP P31327
A	34	GLN	-	expression tag	UNP P31327
A	35	GLY	-	expression tag	UNP P31327
A	36	ALA	-	expression tag	UNP P31327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	UNP P31327
A	38	ASP	-	expression tag	UNP P31327
A	39	PRO	-	expression tag	UNP P31327
B	12	MET	-	initiating methionine	UNP P31327
B	13	SER	-	expression tag	UNP P31327
B	14	TYR	-	expression tag	UNP P31327
B	15	TYR	-	expression tag	UNP P31327
B	16	HIS	-	expression tag	UNP P31327
B	17	HIS	-	expression tag	UNP P31327
B	18	HIS	-	expression tag	UNP P31327
B	19	HIS	-	expression tag	UNP P31327
B	20	HIS	-	expression tag	UNP P31327
B	21	HIS	-	expression tag	UNP P31327
B	22	ASP	-	expression tag	UNP P31327
B	23	TYR	-	expression tag	UNP P31327
B	24	ASP	-	expression tag	UNP P31327
B	25	ILE	-	expression tag	UNP P31327
B	26	PRO	-	expression tag	UNP P31327
B	27	THR	-	expression tag	UNP P31327
B	28	THR	-	expression tag	UNP P31327
B	29	GLU	-	expression tag	UNP P31327
B	30	ASN	-	expression tag	UNP P31327
B	31	LEU	-	expression tag	UNP P31327
B	32	TYR	-	expression tag	UNP P31327
B	33	PHE	-	expression tag	UNP P31327
B	34	GLN	-	expression tag	UNP P31327
B	35	GLY	-	expression tag	UNP P31327
B	36	ALA	-	expression tag	UNP P31327
B	37	MET	-	expression tag	UNP P31327
B	38	ASP	-	expression tag	UNP P31327
B	39	PRO	-	expression tag	UNP P31327

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

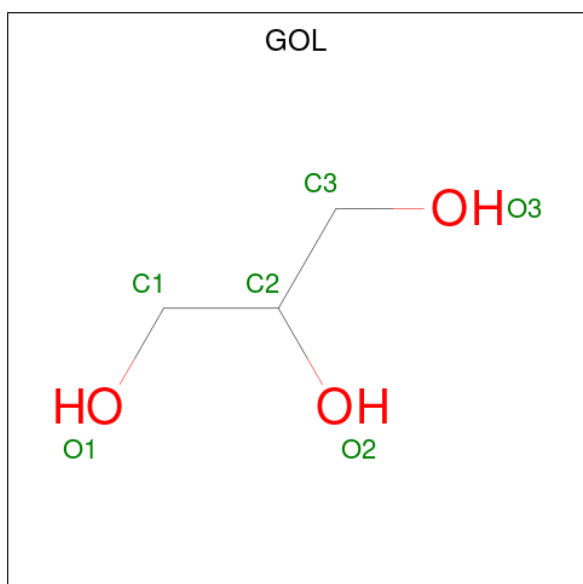
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	B	1	Total Ni 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

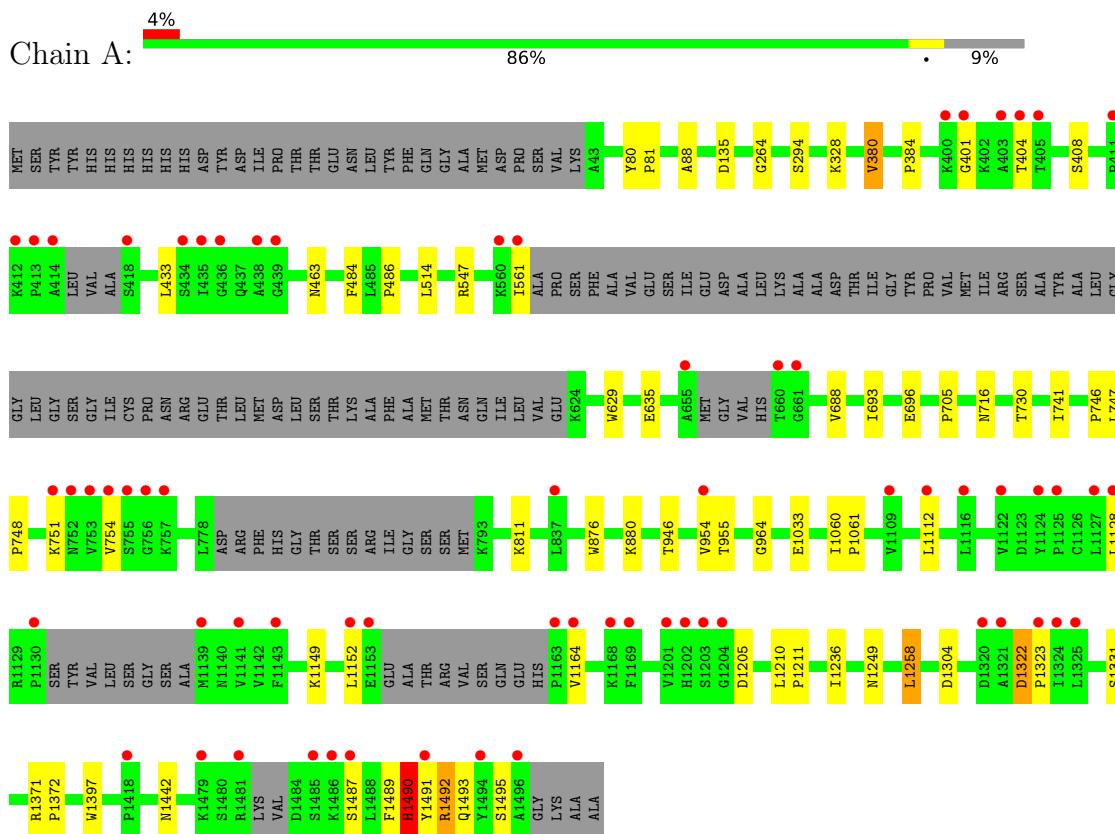
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	398	Total O 398 398	0	0
5	B	421	Total O 421 421	0	0

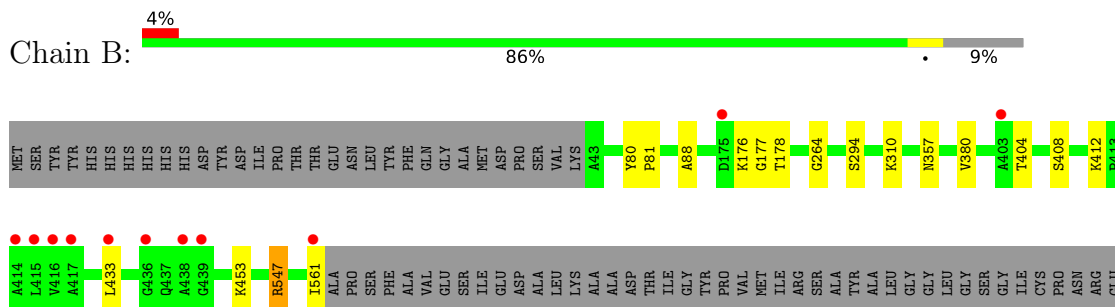
3 Residue-property plots [i](#)

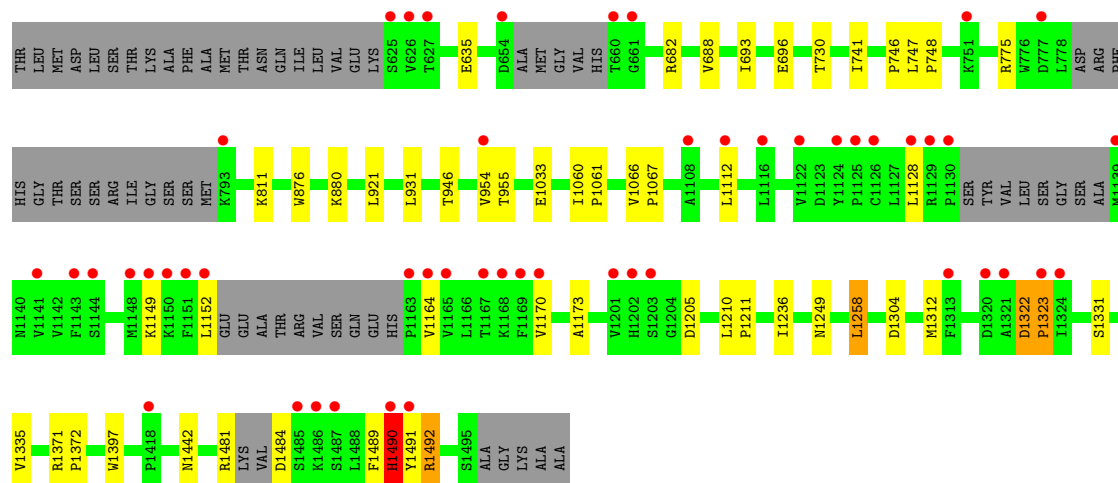
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Carbamoyl-phosphate synthase [ammonia], mitochondrial



- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.34Å 133.48Å 142.91Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	43.95 – 2.40 43.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.95-2.40) 96.1 (43.95-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.165 , 0.196 0.172 , 0.169	Depositor DCC
R_{free} test set	6821 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtrriage
Anisotropy	0.532	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21866	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, EDO, 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	0.71	0/10717	0.80	2/14511 (0.0%)
1	B	0.71	0/10716	0.79	1/14514 (0.0%)
All	All	0.71	0/21433	0.79	3/29025 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1495	SER	N-CA-C	6.29	118.74	108.55
1	B	412	LYS	N-CA-C	-5.95	102.57	110.07
1	A	751	LYS	N-CA-C	5.14	117.88	110.28

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	10503	0	10578	39	0
1	B	10498	0	10576	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	24	1	0
3	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	16	0	0
4	B	12	0	16	1	0
5	A	398	0	0	2	0
5	B	421	0	0	3	0
All	All	21866	0	21216	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 2.

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:A:1487:SER:HA	1:A:1490:HIS:ND1	2.10	0.67
1:B:1492:ARG:HH11	1:B:1492:ARG:HG3	1.60	0.65
1:A:404:THR:HG22	1:A:408:SER:OG	1.97	0.65
1:A:1492:ARG:HH11	1:A:1492:ARG:HG3	1.62	0.64
1:B:1304:ASP:O	1:B:1492:ARG:NH2	2.32	0.63
1:A:88:ALA:HB2	1:A:264:GLY:HA3	1.81	0.62
1:B:357:ASN:ND2	5:B:1702:HOH:O	2.32	0.62
1:B:404:THR:HG22	1:B:408:SER:OG	1.99	0.61
1:B:88:ALA:HB2	1:B:264:GLY:HA3	1.82	0.60
1:A:964:GLY:O	3:A:1602:EDO:H11	2.02	0.60
1:B:178:THR:OG1	1:B:310:LYS:HE2	2.03	0.58
1:B:1492:ARG:HH11	1:B:1492:ARG:CG	2.16	0.58
1:B:1170:VAL:HG23	1:B:1173:ALA:HB2	1.87	0.55
1:A:1304:ASP:O	1:A:1492:ARG:NH2	2.40	0.54
1:B:1170:VAL:CG2	1:B:1173:ALA:HB2	2.38	0.53
1:A:135:ASP:OD1	5:A:1701:HOH:O	2.18	0.53
1:A:401:GLY:HA2	5:A:2042:HOH:O	2.09	0.51
1:A:1371:ARG:HB3	1:A:1397:TRP:CZ2	2.45	0.51
1:A:1322:ASP:N	1:A:1323:PRO:CD	2.75	0.50
1:B:1371:ARG:HB3	1:B:1397:TRP:CZ2	2.46	0.50
1:B:775:ARG:NH2	5:B:1707:HOH:O	2.44	0.50
1:A:754:VAL:HG13	1:A:955:THR:HB	1.94	0.49
1:A:1492:ARG:HD3	1:A:1493:GLN:N	2.27	0.49
1:B:1322:ASP:N	1:B:1323:PRO:CD	2.76	0.49
1:B:931:LEU:HD12	5:B:2036:HOH:O	2.14	0.48
1:A:547:ARG:NH2	1:A:561:ILE:HG21	2.30	0.47
1:A:635:GLU:OE1	1:A:696:GLU:OE2	2.33	0.47
1:A:404:THR:CG2	1:A:408:SER:OG	2.63	0.47
1:A:954:VAL:HG12	1:A:954:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1492:ARG:HG3	1:A:1492:ARG:NH1	2.30	0.47
1:B:1128:LEU:HD11	1:B:1164:VAL:HG11	1.98	0.46
1:A:1060:ILE:HB	1:A:1061:PRO:CD	2.45	0.46
1:B:1205:ASP:HB2	1:B:1331:SER:OG	2.15	0.46
1:B:730:THR:O	1:B:946:THR:HG22	2.16	0.46
1:B:1060:ILE:HB	1:B:1061:PRO:CD	2.46	0.46
1:A:730:THR:O	1:A:946:THR:HG22	2.15	0.45
1:B:404:THR:CG2	1:B:408:SER:OG	2.64	0.45
1:B:876:TRP:CZ2	1:B:880:LYS:HE2	2.52	0.45
1:B:1490:HIS:O	1:B:1491:TYR:C	2.60	0.45
1:A:741:ILE:HD11	1:A:747:LEU:HD21	1.99	0.44
1:A:1128:LEU:HD11	1:A:1164:VAL:HG11	1.99	0.44
1:B:1312:MET:HE2	1:B:1335:VAL:HG13	2.00	0.44
1:A:746:PRO:HB2	1:A:748:PRO:HD2	1.99	0.44
1:B:1492:ARG:HG3	1:B:1492:ARG:NH1	2.30	0.44
1:B:1489:PHE:O	1:B:1491:TYR:N	2.51	0.44
1:B:176:LYS:O	1:B:177:GLY:C	2.61	0.43
1:B:1481:ARG:HG3	1:B:1484:ASP:N	2.32	0.43
1:A:811:LYS:NZ	1:A:1033:GLU:OE2	2.49	0.43
1:B:746:PRO:HB2	1:B:748:PRO:HD2	2.00	0.43
1:B:811:LYS:NZ	1:B:1033:GLU:OE2	2.50	0.43
1:B:954:VAL:HG12	1:B:954:VAL:O	2.18	0.43
1:A:688:VAL:HG13	1:A:693:ILE:HB	2.01	0.43
1:A:514:LEU:C	1:A:514:LEU:HD23	2.44	0.43
1:A:876:TRP:CZ2	1:A:880:LYS:HE2	2.54	0.43
1:A:1205:ASP:HB2	1:A:1331:SER:OG	2.18	0.43
1:A:1371:ARG:HB2	1:A:1372:PRO:HD3	2.01	0.43
1:B:635:GLU:OE2	1:B:696:GLU:OE2	2.36	0.43
1:A:486:PRO:HD3	1:A:1489:PHE:CE2	2.54	0.43
1:A:1490:HIS:O	1:A:1491:TYR:C	2.62	0.42
1:A:1489:PHE:O	1:A:1491:TYR:N	2.53	0.42
1:B:1112:LEU:HD21	1:B:1149:LYS:HG3	2.02	0.42
1:A:1236:ILE:HD11	1:A:1258:LEU:HD11	2.02	0.42
1:B:1066:VAL:HB	1:B:1067:PRO:HD3	2.02	0.42
1:A:80:TYR:N	1:A:81:PRO:CD	2.83	0.42
1:A:1060:ILE:HB	1:A:1061:PRO:HD3	2.00	0.42
1:A:463:ASN:O	1:A:484:PHE:HA	2.20	0.42
1:B:80:TYR:N	1:B:81:PRO:CD	2.83	0.42
1:B:741:ILE:HD11	1:B:747:LEU:HD21	2.01	0.41
1:B:921:LEU:O	4:B:1604:GOL:H2	2.20	0.41
1:B:547:ARG:NH2	1:B:561:ILE:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1236:ILE:HD11	1:B:1258:LEU:HD11	2.02	0.41
1:A:1112:LEU:HD21	1:A:1149:LYS:HG3	2.02	0.41
1:B:1371:ARG:HB2	1:B:1372:PRO:HD3	2.02	0.41
1:B:1210:LEU:HD12	1:B:1211:PRO:HA	2.03	0.41
1:B:1060:ILE:HB	1:B:1061:PRO:HD3	2.02	0.41
1:B:682:ARG:HD2	1:B:682:ARG:HA	1.77	0.41
1:B:688:VAL:HG13	1:B:693:ILE:HB	2.03	0.41
1:A:1210:LEU:HD12	1:A:1211:PRO:HA	2.03	0.41
1:A:629:TRP:HA	1:A:705:PRO:HD3	2.03	0.40
1:B:1205:ASP:CB	1:B:1331:SER:OG	2.69	0.40
1:A:380:VAL:HG11	1:A:384:PRO:O	2.21	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	1340/1489 (90%)	1296 (97%)	39 (3%)	5 (0%)	30 43
1	B	1342/1489 (90%)	1295 (96%)	41 (3%)	6 (0%)	30 43
All	All	2682/2978 (90%)	2591 (97%)	80 (3%)	11 (0%)	30 43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1322	ASP
1	A	1490	HIS
1	B	1322	ASP
1	B	1490	HIS
1	A	380	VAL
1	A	1442	ASN
1	B	380	VAL

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Mol	Chain	Res	Type
1	B	1442	ASN
1	A	294	SER
1	B	294	SER
1	B	1323	PRO

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	1159/1266 (92%)	1151 (99%)	8 (1%)	76	88
1	B	1160/1266 (92%)	1151 (99%)	9 (1%)	73	86
All	All	2319/2532 (92%)	2302 (99%)	17 (1%)	76	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	433	LEU
1	A	716	ASN
1	A	1152	LEU
1	A	1249	ASN
1	A	1258	LEU
1	A	1490	HIS
1	A	1492	ARG
1	B	433	LEU
1	B	453	LYS
1	B	547	ARG
1	B	955	THR
1	B	1152	LEU
1	B	1249	ASN
1	B	1258	LEU
1	B	1490	HIS
1	B	1492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	HIS
1	A	985	HIS
1	A	1110	ASN
1	A	1202	HIS
1	A	1292	HIS
1	A	1359	GLN
1	A	1416	GLN
1	A	1447	HIS
1	B	357	ASN
1	B	359	GLN
1	B	985	HIS
1	B	1140	ASN
1	B	1243	GLN
1	B	1292	HIS
1	B	1447	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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
4	GOL	A	1605	-	5,5,5	0.49	0	5,5,5	0.24	0
3	EDO	B	1602	-	3,3,3	0.71	0	2,2,2	0.31	0
4	GOL	B	1604	-	5,5,5	0.68	0	5,5,5	0.71	0
4	GOL	A	1607	-	5,5,5	0.64	0	5,5,5	0.47	0
3	EDO	A	1603	-	3,3,3	0.71	0	2,2,2	0.35	0
3	EDO	A	1604	-	3,3,3	0.48	0	2,2,2	0.52	0
3	EDO	A	1602	-	3,3,3	0.74	0	2,2,2	0.24	0
3	EDO	A	1606	-	3,3,3	0.85	0	2,2,2	0.62	0
4	GOL	B	1603	-	5,5,5	0.59	0	5,5,5	0.58	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
4	GOL	A	1605	-	-	2/4/4/4	-
3	EDO	B	1602	-	-	1/1/1/1	-
4	GOL	B	1604	-	-	0/4/4/4	-
4	GOL	A	1607	-	-	4/4/4/4	-
3	EDO	A	1603	-	-	0/1/1/1	-
3	EDO	A	1604	-	-	1/1/1/1	-
3	EDO	A	1602	-	-	1/1/1/1	-
3	EDO	A	1606	-	-	0/1/1/1	-
4	GOL	B	1603	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1605	GOL	C1-C2-C3-O3
4	A	1607	GOL	O1-C1-C2-C3
4	A	1607	GOL	C1-C2-C3-O3
4	A	1607	GOL	O2-C2-C3-O3
4	B	1603	GOL	O1-C1-C2-C3
4	B	1603	GOL	C1-C2-C3-O3
4	A	1605	GOL	O2-C2-C3-O3
4	B	1603	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1607	GOL	O1-C1-C2-O2
4	B	1603	GOL	O2-C2-C3-O3
3	A	1604	EDO	O1-C1-C2-O2
3	B	1602	EDO	O1-C1-C2-O2
3	A	1602	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	GOL	1	0
3	A	1602	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	1352/1489 (90%)	-0.20	65 (4%) 35 32	14, 34, 90, 174	4 (0%)
1	B	1351/1489 (90%)	-0.23	61 (4%) 38 34	13, 32, 92, 160	5 (0%)
All	All	2703/2978 (90%)	-0.22	126 (4%) 36 32	13, 33, 91, 174	9 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1152	LEU	7.0
1	B	1201	VAL	6.9
1	A	1201	VAL	6.5
1	B	1163	PRO	5.7
1	A	1202	HIS	5.0
1	B	1130	PRO	4.9
1	A	1321	ALA	4.8
1	A	1496	ALA	4.7
1	B	403	ALA	4.7
1	A	660	THR	4.6
1	B	1323	PRO	4.6
1	A	1163	PRO	4.6
1	A	413	PRO	4.5
1	A	1152	LEU	4.3
1	B	1143	PHE	4.2
1	A	655	ALA	4.2
1	B	954	VAL	4.1
1	B	1151	PHE	4.1
1	B	1202	HIS	3.9
1	A	753	VAL	3.9
1	A	1130	PRO	3.9
1	A	1491	TYR	3.9
1	B	660	THR	3.8
1	B	1491	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	438	ALA	3.8
1	A	1323	PRO	3.8
1	A	755	SER	3.6
1	B	417	ALA	3.6
1	B	1486	LYS	3.5
1	A	1139	MET	3.5
1	A	1486	LYS	3.5
1	A	439	GLY	3.5
1	A	1324	ILE	3.4
1	B	1144	SER	3.4
1	B	433	LEU	3.3
1	B	1321	ALA	3.3
1	A	661	GLY	3.3
1	B	561	ILE	3.3
1	A	1485	SER	3.3
1	A	414	ALA	3.2
1	A	754	VAL	3.2
1	B	416	VAL	3.2
1	B	1139	MET	3.1
1	A	418	SER	3.1
1	B	415	LEU	3.1
1	A	1112	LEU	3.0
1	A	561	ILE	3.0
1	B	1112	LEU	3.0
1	A	1481	ARG	3.0
1	B	1122	VAL	2.9
1	A	403	ALA	2.9
1	B	175	ASP	2.9
1	B	1124	TYR	2.9
1	B	1324	ILE	2.8
1	B	1169	PHE	2.8
1	A	1487	SER	2.8
1	A	435	ILE	2.8
1	B	1203	SER	2.8
1	A	1164	VAL	2.8
1	A	434	SER	2.7
1	A	1320	ASP	2.7
1	B	777	ASP	2.7
1	A	1125	PRO	2.7
1	B	1128	LEU	2.7
1	B	414	ALA	2.7
1	B	1485	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	752	ASN	2.7
1	B	1125	PRO	2.6
1	B	1490	HIS	2.6
1	B	439	GLY	2.6
1	A	436	GLY	2.6
1	A	1116	LEU	2.6
1	B	1165	VAL	2.6
1	A	1203	SER	2.6
1	B	438	ALA	2.5
1	A	1122	VAL	2.5
1	B	1141	VAL	2.5
1	B	1148	MET	2.5
1	A	1418	PRO	2.5
1	A	1169	PHE	2.5
1	A	411	PRO	2.4
1	B	1108	ALA	2.4
1	B	1150	LYS	2.4
1	A	954	VAL	2.4
1	B	1418	PRO	2.4
1	B	1126	CYS	2.4
1	B	1487	SER	2.4
1	A	1128	LEU	2.4
1	A	1141	VAL	2.4
1	B	626	VAL	2.4
1	B	1164	VAL	2.4
1	A	757	LYS	2.4
1	A	756	GLY	2.3
1	A	837	LEU	2.3
1	A	1143	PHE	2.3
1	B	793	LYS	2.3
1	A	1124	TYR	2.3
1	B	661	GLY	2.3
1	B	1320	ASP	2.3
1	A	1153	GLU	2.2
1	A	401	GLY	2.2
1	A	751	LYS	2.2
1	A	1479	LYS	2.2
1	B	1168	LYS	2.2
1	B	1170	VAL	2.2
1	A	1204	GLY	2.2
1	B	1116	LEU	2.2
1	B	654	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1313	PHE	2.2
1	A	405	THR	2.1
1	A	1127	LEU	2.1
1	B	436	GLY	2.1
1	B	1129	ARG	2.1
1	A	400	LYS	2.1
1	A	1109	VAL	2.1
1	A	1325	LEU	2.1
1	B	627	THR	2.1
1	B	625	SER	2.1
1	A	412	LYS	2.1
1	A	404	THR	2.1
1	A	560	LYS	2.1
1	A	1168	LYS	2.0
1	B	751	LYS	2.0
1	B	1149	LYS	2.0
1	B	1167	THR	2.0
1	A	1494	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(\AA^2)	Q<0.9
4	GOL	B	1603	6/6	0.76	0.17	58,65,69,69	0
3	EDO	A	1606	4/4	0.78	0.24	40,44,48,54	0
3	EDO	A	1602	4/4	0.81	0.18	44,47,56,62	0
4	GOL	A	1607	6/6	0.84	0.19	48,65,82,84	0
4	GOL	A	1605	6/6	0.85	0.15	48,55,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	1603	4/4	0.87	0.17	34,45,46,47	0
4	GOL	B	1604	6/6	0.91	0.12	53,57,62,66	0
3	EDO	A	1604	4/4	0.93	0.10	40,43,44,45	0
3	EDO	B	1602	4/4	0.95	0.11	40,41,46,46	0
2	NI	B	1601	1/1	1.00	0.02	32,32,32,32	0
2	NI	A	1601	1/1	1.00	0.05	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.