Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 01:55 pm GMT

PDB ID	:	5DOT
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 (i) 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 (i)) were used in the production of this report:

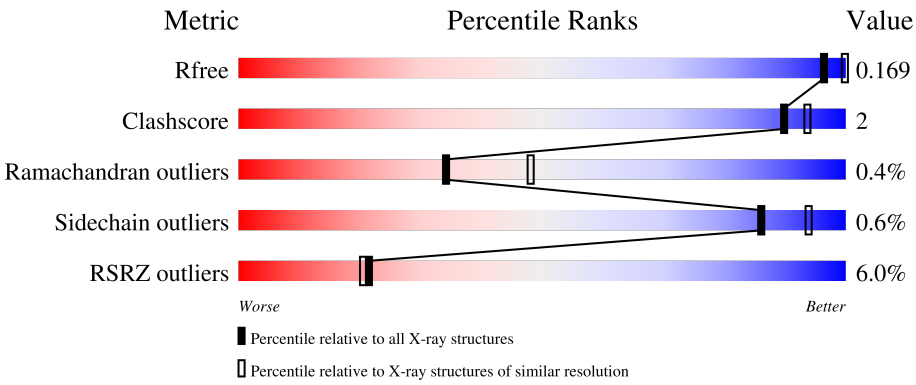
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	6% 86% • 9%
1	B	1489	5% 86% • 9%

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
4	GOL	A	1607	-	-	-	X

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

Continued on next page...

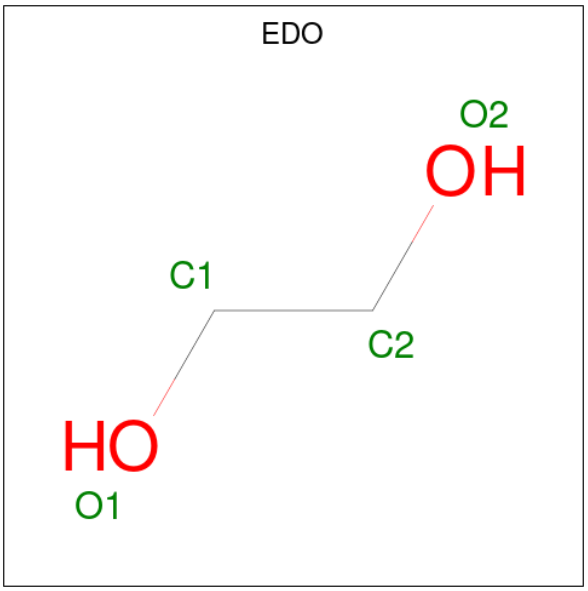
Continued from previous page...

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 (three-letter code: NI) (formula: Ni).

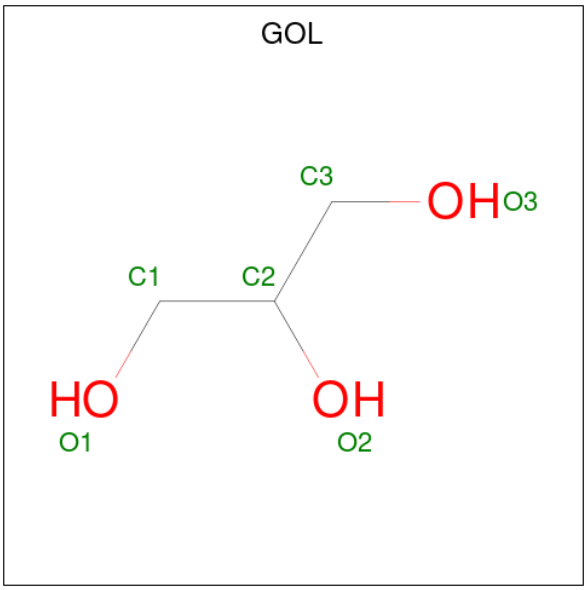
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	1	1	1	0	0
			Total	Ni		
2	B	1	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

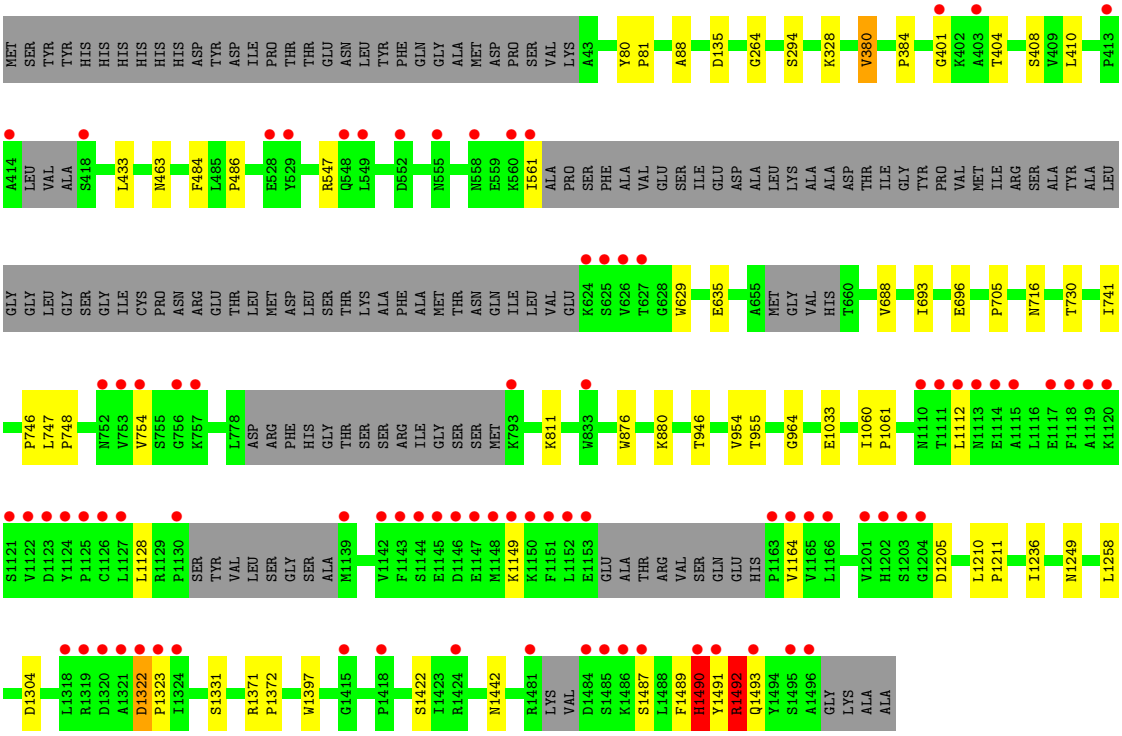
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	398	398	398	0	0
			Total	O		
5	B	421	421	421	0	0

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.

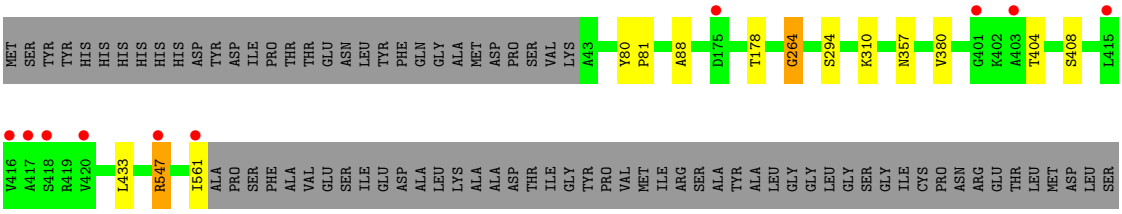
• Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

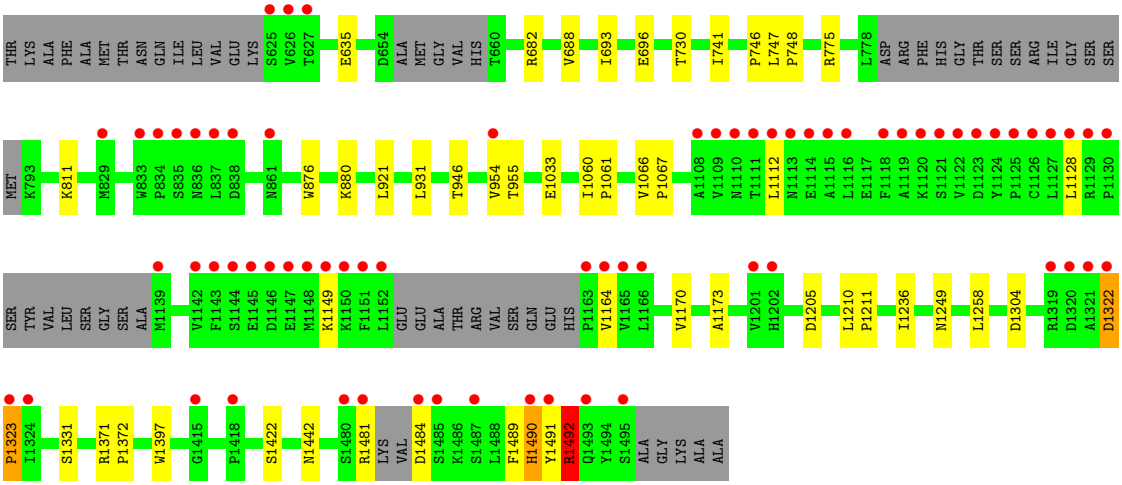
Chain A:



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

Chain B:




THR LYS ALA PHE ALA MET THR ASN GLN ILE LEU VAL GLU LYS S625 V626 T627 E635 D654 ALA MET GLY VAL HIS T660 R682 V688 I693 E696 T730 I741 P746 L747 P748 R775 L778 ASP ARG PHE HIS GLY THR SER SER ARG ILE GLY SER SER
MET K793 K811 N829 W833 P834 S835 N836 L837 D838 N861 W876 K880 L921 L931 T946 V954 T955 E1033 I1060 P1061 V1066 P1067 A1108 V1109 N1110 T1111 L1112 N1113 E1114 A1115 L1116 E1117 F1118 A1119 K1120 S1121 V1122 D1123 Y1124 P1125 C1126 L1127 L1128 R1129 P1130
SER TYR VAL LEU SER GLY SER ALA M1139 V1142 F1143 S1144 E1145 D1146 E1147 M1148 K1149 K1150 F1151 L1152 GLU GLU ALA THR ARG VAL SER GLN GLU HIS P1163 V1164 V1165 L1166 V1170 A1173 V1201 H1202 D1205 L1210 P1211 I1236 N1249 L1258 D1304 R1319 D1320 A1321 D1322
P1323 I1324 S1331 R1371 P1372 W1397 G1415 P1418 S1422 N1442 S1480 R1481 LYS VAL D1484 S1485 K1486 S1487 L1488 F1489 H1490 Y1491 R1492 Q1493 Y1494 S1495 ALA GLY LYS ALA ALA

4 Data and refinement statistics (i)

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 43.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.95-2.40) 96.1 (43.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.39Å)	Xtriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, EDO, NI

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	0.50	0/10717	0.65	3/14511 (0.0%)
1	B	0.51	1/10716 (0.0%)	0.65	1/14514 (0.0%)
All	All	0.51	1/21433 (0.0%)	0.65	4/29025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	GLY	N-CA	-5.17	1.38	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1492	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	1492	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	410	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	1492	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10498	0	10576	39	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
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	76	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 (76) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:811:LYS:NZ	1:B:1033:GLU:OE2	2.50	0.45
1:B:876:TRP:CZ2	1:B:880:LYS:HE2	2.52	0.45
1:A:741:ILE:HD11	1:A:747:LEU:HD21	1.99	0.44
1:A:811:LYS:NZ	1:A:1033:GLU:OE2	2.49	0.44
1:A:1128:LEU:HD11	1:A:1164:VAL:HG11	1.99	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:1481:ARG:HG3	1:B:1484:ASP:N	2.32	0.43
1:B:746:PRO:HB2	1:B:748:PRO:HD2	2.00	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: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: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

Continued on next page...

Continued from previous page...

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%)	34	48
1	B	1342/1489 (90%)	1295 (96%)	41 (3%)	6 (0%)	34	48
All	All	2682/2978 (90%)	2591 (97%)	80 (3%)	11 (0%)	34	48

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

Continued on next page...

Continued from previous page...

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%)	1152 (99%)	7 (1%)	86	94
1	B	1160/1266 (92%)	1153 (99%)	7 (1%)	86	94
All	All	2319/2532 (92%)	2305 (99%)	14 (1%)	86	94

All (14) 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	1249	ASN
1	A	1422	SER
1	A	1490	HIS
1	A	1492	ARG
1	B	433	LEU
1	B	547	ARG
1	B	955	THR
1	B	1249	ASN
1	B	1422	SER
1	B	1490	HIS
1	B	1492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1103	GLN
1	B	154	GLN

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 monosaccharides 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	1607	-	5,5,5	0.61	0	5,5,5	0.47	0
3	EDO	A	1603	-	3,3,3	0.76	0	2,2,2	0.44	0
4	GOL	B	1603	-	5,5,5	0.57	0	5,5,5	0.57	0
3	EDO	A	1604	-	3,3,3	0.51	0	2,2,2	0.51	0
4	GOL	A	1605	-	5,5,5	0.48	0	5,5,5	0.25	0
4	GOL	B	1604	-	5,5,5	0.66	0	5,5,5	0.69	0
3	EDO	A	1602	-	3,3,3	0.77	0	2,2,2	0.32	0
3	EDO	A	1606	-	3,3,3	0.89	0	2,2,2	0.72	0
3	EDO	B	1602	-	3,3,3	0.74	0	2,2,2	0.38	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	1607	-	-	4/4/4/4	-
3	EDO	A	1603	-	-	0/1/1/1	-
4	GOL	B	1603	-	-	4/4/4/4	-
3	EDO	A	1604	-	-	1/1/1/1	-
4	GOL	A	1605	-	-	2/4/4/4	-
4	GOL	B	1604	-	-	0/4/4/4	-
3	EDO	A	1602	-	-	1/1/1/1	-
3	EDO	A	1606	-	-	0/1/1/1	-
3	EDO	B	1602	-	-	1/1/1/1	-

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
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 (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	1352/1489 (90%)	-0.00	84 (6%)	20	19	17, 34, 90, 174	0
1	B	1351/1489 (90%)	-0.10	79 (5%)	23	22	15, 32, 92, 160	0
All	All	2703/2978 (90%)	-0.05	163 (6%)	21	20	15, 33, 91, 174	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1321	ALA	12.7
1	B	1201	VAL	10.2
1	A	1320	ASP	9.7
1	B	1320	ASP	8.9
1	B	1323	PRO	8.1
1	B	1321	ALA	7.6
1	B	1151	PHE	7.0
1	A	1152	LEU	6.8
1	A	1151	PHE	6.5
1	B	1112	LEU	6.2
1	A	1491	TYR	6.0
1	A	1153	GLU	5.7
1	B	403	ALA	5.6
1	A	1112	LEU	5.6
1	B	1143	PHE	5.4
1	B	626	VAL	5.3
1	A	414	ALA	5.3
1	A	1324	ILE	5.3
1	B	1164	VAL	5.3
1	A	1201	VAL	5.2
1	B	1324	ILE	5.2
1	B	1124	TYR	5.1
1	A	1118	PHE	5.0
1	B	1152	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1144	SER	4.7
1	A	1124	TYR	4.7
1	A	401	GLY	4.7
1	B	1322	ASP	4.6
1	B	1148	MET	4.6
1	A	756	GLY	4.5
1	A	1164	VAL	4.4
1	B	1165	VAL	4.4
1	B	1149	LYS	4.2
1	A	1323	PRO	4.2
1	B	417	ALA	4.2
1	A	1484	ASP	4.2
1	B	1146	ASP	4.2
1	B	1484	ASP	4.2
1	A	1149	LYS	4.1
1	A	1143	PHE	4.0
1	B	1118	PHE	4.0
1	A	1485	SER	3.9
1	B	625	SER	3.9
1	B	1128	LEU	3.9
1	A	1148	MET	3.9
1	A	1122	VAL	3.9
1	B	1122	VAL	3.9
1	A	1490	HIS	3.9
1	A	560	LYS	3.9
1	B	1109	VAL	3.9
1	A	1481	ARG	3.8
1	B	1485	SER	3.8
1	B	175	ASP	3.8
1	B	1130	PRO	3.8
1	B	416	VAL	3.8
1	B	1491	TYR	3.8
1	B	415	LEU	3.7
1	A	1130	PRO	3.7
1	A	1487	SER	3.7
1	A	1493	GLN	3.7
1	B	401	GLY	3.6
1	B	627	THR	3.6
1	B	1163	PRO	3.6
1	A	1115	ALA	3.6
1	A	1146	ASP	3.6
1	A	1322	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1110	ASN	3.5
1	A	1150	LYS	3.5
1	B	1493	GLN	3.5
1	A	625	SER	3.5
1	A	1203	SER	3.5
1	A	1121	SER	3.4
1	A	1126	CYS	3.4
1	B	1166	LEU	3.4
1	A	1418	PRO	3.4
1	B	1129	ARG	3.3
1	B	837	LEU	3.3
1	A	1111	THR	3.3
1	A	1142	VAL	3.3
1	A	418	SER	3.2
1	B	1111	THR	3.2
1	B	1147	GLU	3.2
1	A	1495	SER	3.2
1	A	1145	GLU	3.2
1	A	413	PRO	3.2
1	B	1139	MET	3.1
1	B	418	SER	3.1
1	B	561	ILE	3.1
1	A	1415	GLY	3.0
1	B	1126	CYS	3.0
1	A	548	GLN	3.0
1	A	1163	PRO	3.0
1	A	1120	LYS	3.0
1	B	1150	LYS	3.0
1	B	1114	GLU	2.9
1	A	555	ASN	2.9
1	B	1202	HIS	2.9
1	A	753	VAL	2.9
1	B	1123	ASP	2.8
1	B	836	ASN	2.8
1	B	1142	VAL	2.8
1	B	1119	ALA	2.8
1	A	1123	ASP	2.8
1	A	1147	GLU	2.8
1	A	552	ASP	2.8
1	B	1108	ALA	2.7
1	B	1490	HIS	2.7
1	A	1318	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	793	LYS	2.7
1	B	1125	PRO	2.7
1	A	752	ASN	2.7
1	A	561	ILE	2.7
1	B	1121	SER	2.7
1	B	1495	SER	2.7
1	B	1319	ARG	2.7
1	B	834	PRO	2.6
1	A	1119	ALA	2.6
1	A	1204	GLY	2.6
1	A	757	LYS	2.6
1	B	1115	ALA	2.6
1	A	1117	GLU	2.6
1	A	1165	VAL	2.5
1	B	954	VAL	2.5
1	A	1202	HIS	2.5
1	B	829	MET	2.5
1	A	626	VAL	2.5
1	A	833	TRP	2.5
1	A	1496	ALA	2.5
1	B	1113	ASN	2.4
1	B	838	ASP	2.4
1	B	1145	GLU	2.4
1	A	627	THR	2.4
1	B	1144	SER	2.4
1	A	624	LYS	2.4
1	A	1127	LEU	2.4
1	A	1110	ASN	2.3
1	B	861	ASN	2.3
1	B	1418	PRO	2.3
1	A	529	TYR	2.3
1	B	1415	GLY	2.3
1	A	1319	ARG	2.3
1	B	1120	LYS	2.3
1	A	1125	PRO	2.3
1	B	835	SER	2.3
1	A	1166	LEU	2.3
1	A	1139	MET	2.3
1	A	403	ALA	2.3
1	B	1481	ARG	2.2
1	A	558	ASN	2.2
1	B	420	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	528	GLU	2.2
1	B	1127	LEU	2.2
1	B	833	TRP	2.2
1	B	1480	SER	2.2
1	A	1486	LYS	2.1
1	A	1114	GLU	2.1
1	A	1113	ASN	2.1
1	A	1424	ARG	2.1
1	B	1116	LEU	2.1
1	B	1487	SER	2.0
1	A	754	VAL	2.0
1	A	549	LEU	2.0
1	B	547	ARG	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 monosaccharides 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	EDO	A	1602	4/4	0.73	0.32	44,47,56,62	0
3	EDO	A	1606	4/4	0.74	0.25	40,44,48,54	0
4	GOL	A	1607	6/6	0.78	0.43	48,65,82,84	0
4	GOL	A	1605	6/6	0.82	0.18	48,55,65,66	0
3	EDO	A	1603	4/4	0.84	0.23	34,45,46,47	0
4	GOL	B	1603	6/6	0.84	0.17	58,65,69,69	0
4	GOL	B	1604	6/6	0.86	0.19	53,57,62,66	0
3	EDO	B	1602	4/4	0.93	0.19	40,41,46,46	0
3	EDO	A	1604	4/4	0.94	0.17	40,43,44,45	0
2	NI	B	1601	1/1	1.00	0.08	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.