Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:14 PM GMT

PDB ID	:	4O90
Title	:	Crystal structure of chorismate synthase from Acinetobacter baumannii at 2.6A resolution
Authors	:	Chaudhary, A.; Singh, N.; Shukla, P.K.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2013-12-31
Resolution	:	2.61 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

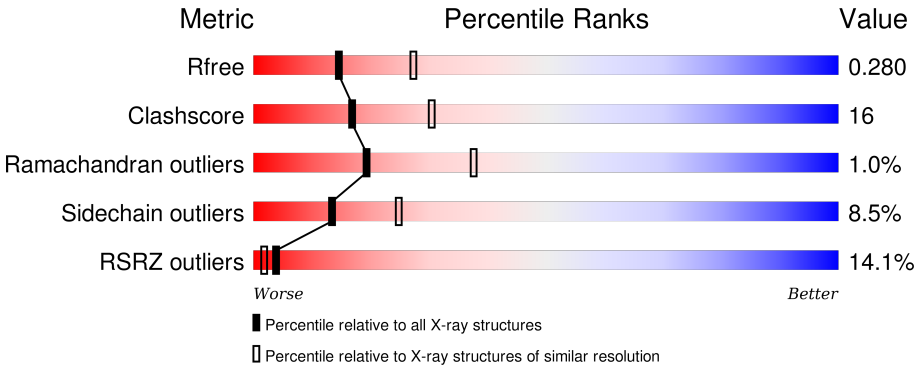
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.61 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}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	363	10% 54% 24% • • 19%
1	B	363	12% 55% 22% • 19%

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
3	GOL	B	402	-	-	-	X

2 Entry composition

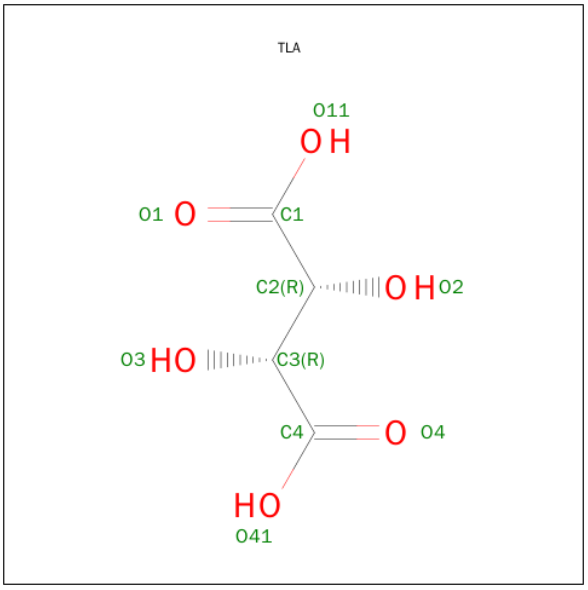
There are 4 unique types of molecules in this entry. The entry contains 4600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chorismate synthase.

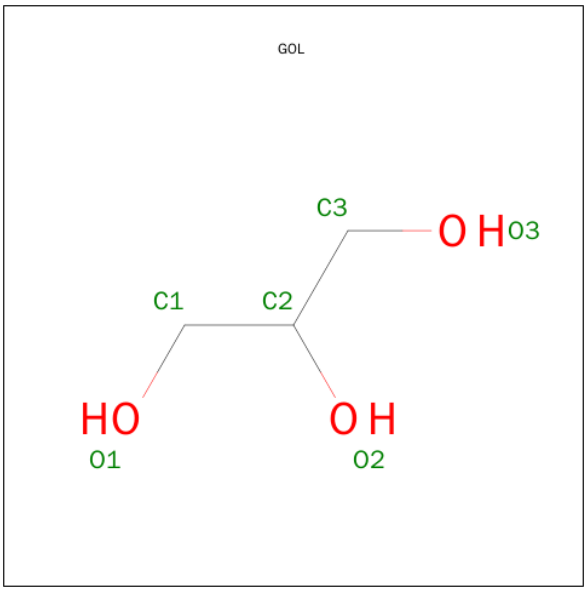
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2200	1376	397	416	11			
1	B	294	Total	C	N	O	S	0	0	0
			2200	1376	397	416	11			

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

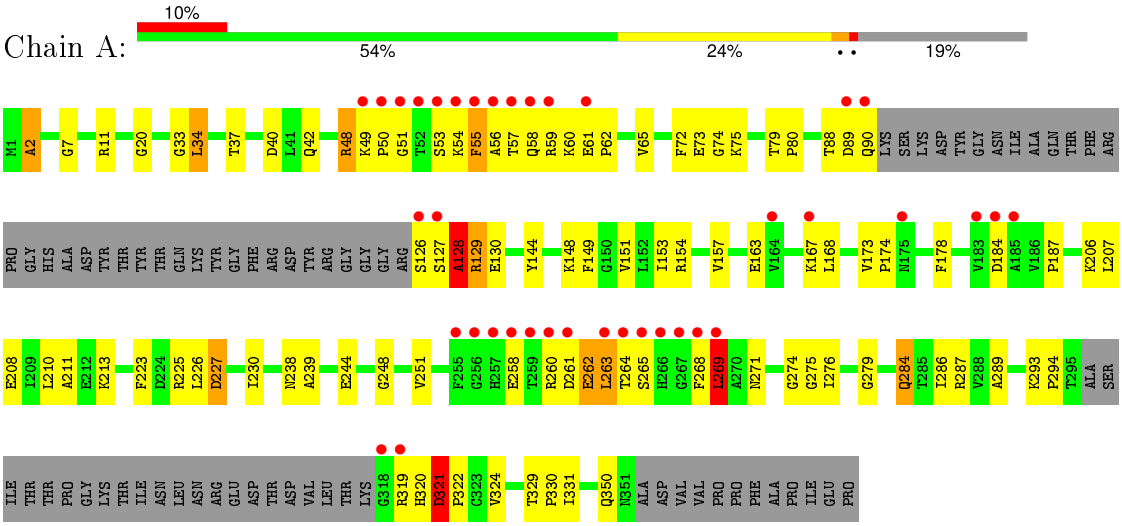
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total O 81 81	0	0
4	B	87	Total O 87 87	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

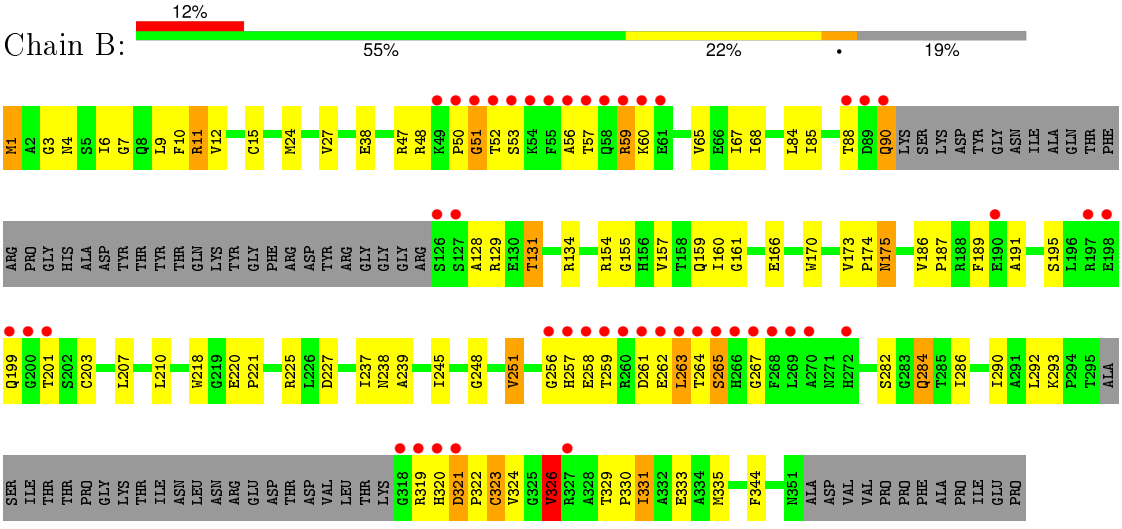
- Molecule 1: Chorismate synthase

Chain A:



- Molecule 1: Chorismate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	108.74Å 73.19Å 90.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.37 – 2.61 32.37 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.3 (32.37-2.61) 93.3 (32.37-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.279 0.261 , 0.280	Depositor DCC
R_{free} test set	1026 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	3 of 21001 reflections (0.014%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4600	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, TLA

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	1.00	1/2236 (0.0%)	1.00	3/3021 (0.1%)
1	B	0.85	0/2236	1.01	9/3021 (0.3%)
All	All	0.93	1/4472 (0.0%)	1.00	12/6042 (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	A	0	4
1	B	0	3
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	GLU	CD-OE1	-5.09	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	GLY	N-CA-C	-6.84	96.01	113.10
1	B	264	THR	N-CA-C	6.57	128.72	111.00
1	B	4	ASN	N-CA-C	6.38	128.23	111.00
1	A	321	ASP	C-N-CD	-6.17	107.03	120.60
1	B	321	ASP	N-CA-C	-5.85	95.20	111.00
1	A	33	GLY	N-CA-C	5.82	127.66	113.10
1	B	326	VAL	CB-CA-C	-5.75	100.48	111.40
1	B	282	SER	CB-CA-C	-5.74	99.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	ASP	C-N-CD	-5.65	108.17	120.60
1	B	9	LEU	CB-CG-CD1	-5.33	101.95	111.00
1	B	267	GLY	N-CA-C	5.24	126.19	113.10
1	A	128	ALA	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ALA	Peptide
1	A	2	ALA	Peptide
1	A	269	LEU	Peptide
1	A	53	SER	Peptide
1	B	256	GLY	Peptide
1	B	265	SER	Peptide
1	B	321	ASP	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	2200	0	2203	73	0
1	B	2200	0	2203	73	0
2	A	10	0	4	2	0
2	B	10	0	4	1	0
3	A	6	0	8	0	0
3	B	6	0	8	2	0
4	A	81	0	0	2	0
4	B	87	0	0	5	0
All	All	4600	0	4430	145	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 16.

All (145) 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:60:LYS:HG3	1:A:61:GLU:H	1.23	1.04
1:A:225:ARG:HG2	1:A:279:GLY:HA3	1.44	0.97
1:B:90:GLN:HA	1:B:90:GLN:OE1	1.74	0.87
1:B:237:ILE:HG12	1:B:331:ILE:HD11	1.62	0.82
1:A:51:GLY:CA	1:A:54:LYS:HB3	2.10	0.82
1:A:49:LYS:O	1:A:49:LYS:HG3	1.79	0.81
1:B:186:VAL:HB	1:B:187:PRO:HD3	1.62	0.80
1:A:48:ARG:O	1:A:50:PRO:HD3	1.82	0.79
1:A:261:ASP:O	1:A:262:GLU:OE2	2.01	0.79
1:A:271:ASN:HD21	1:A:284:GLN:HB2	1.48	0.78
1:B:90:GLN:CA	1:B:90:GLN:OE1	2.30	0.78
1:B:238:ASN:O	1:B:239:ALA:HB3	1.82	0.77
1:A:268:PHE:CD2	1:A:268:PHE:O	2.37	0.76
1:B:290:ILE:HD12	1:B:292:LEU:HD11	1.69	0.74
1:B:237:ILE:HG12	1:B:331:ILE:CD1	2.19	0.73
1:A:51:GLY:HA2	1:A:54:LYS:HB3	1.70	0.73
1:A:20:GLY:HA3	4:A:517:HOH:O	1.89	0.73
1:A:293:LYS:HA	1:B:251:VAL:HG13	1.69	0.72
1:B:323:CYS:O	1:B:326:VAL:HG22	1.92	0.69
1:B:323:CYS:O	1:B:326:VAL:CG2	2.41	0.68
1:A:60:LYS:HG3	1:A:61:GLU:N	2.01	0.67
1:B:237:ILE:CG1	1:B:331:ILE:HD11	2.24	0.67
1:A:184:ASP:O	1:A:187:PRO:HG2	1.96	0.66
1:A:58:GLN:HG3	1:A:59:ARG:H	1.61	0.66
1:B:262:GLU:HG2	1:B:263:LEU:HG	1.77	0.65
1:A:223:PHE:HB3	1:B:6:ILE:HD13	1.79	0.64
1:A:261:ASP:O	1:A:262:GLU:CD	2.36	0.64
1:B:238:ASN:O	1:B:239:ALA:CB	2.45	0.63
1:B:186:VAL:N	1:B:187:PRO:CD	2.59	0.63
1:B:53:SER:O	1:B:59:ARG:NH2	2.31	0.63
1:B:38:GLU:HG3	1:B:67:ILE:HG13	1.80	0.63
1:A:54:LYS:HG3	1:A:55:PHE:H	1.62	0.63
1:A:211:ALA:HB3	1:A:286:ILE:HB	1.81	0.62
1:A:55:PHE:CD2	1:A:56:ALA:N	2.66	0.62
1:A:49:LYS:O	1:A:49:LYS:CG	2.47	0.62
1:B:186:VAL:CB	1:B:187:PRO:HD3	2.30	0.61
1:B:290:ILE:CD1	1:B:292:LEU:HD11	2.31	0.61
1:B:257:HIS:CD2	1:B:259:THR:HG22	2.35	0.61
1:A:65:VAL:O	1:A:65:VAL:HG13	1.99	0.61
1:A:268:PHE:CG	1:A:268:PHE:O	2.51	0.61
1:A:51:GLY:HA3	1:A:54:LYS:HB3	1.83	0.60
1:A:321:ASP:HB3	1:A:324:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:THR:HB	1:B:330:PRO:HD3	1.84	0.60
1:A:51:GLY:HA2	1:A:54:LYS:CB	2.31	0.59
1:B:261:ASP:OD1	1:B:262:GLU:N	2.34	0.59
1:A:226:LEU:O	1:A:230:ILE:HG12	2.03	0.58
1:B:248:GLY:O	1:B:251:VAL:HB	2.02	0.58
1:B:175:ASN:N	1:B:175:ASN:OD1	2.36	0.57
1:A:238:ASN:O	1:A:239:ALA:HB3	2.04	0.57
1:A:261:ASP:HA	4:A:573:HOH:O	2.04	0.57
1:B:48:ARG:NH1	1:B:128:ALA:O	2.37	0.57
1:B:262:GLU:O	1:B:263:LEU:HB2	2.05	0.56
1:A:58:GLN:HG3	1:A:59:ARG:N	2.21	0.55
1:B:160:ILE:CG2	1:B:203:CYS:SG	2.95	0.54
1:A:293:LYS:HB2	1:A:294:PRO:HD2	1.90	0.54
1:A:227:ASP:OD1	1:A:227:ASP:N	2.36	0.54
1:B:60:LYS:HG3	1:B:60:LYS:O	2.07	0.54
1:A:127:SER:C	1:A:129:ARG:HB2	2.29	0.53
1:A:57:THR:OG1	1:A:58:GLN:N	2.40	0.53
2:A:401:TLA:O3	2:A:401:TLA:O11	2.23	0.52
1:A:55:PHE:CG	1:A:56:ALA:N	2.78	0.52
1:B:186:VAL:N	1:B:187:PRO:HD2	2.24	0.52
1:B:157:VAL:HG21	1:B:326:VAL:HG12	1.91	0.52
1:B:160:ILE:HG22	1:B:203:CYS:SG	2.49	0.51
1:B:15:CYS:SG	1:B:24:MET:HB2	2.50	0.51
1:B:319:ARG:HD2	4:B:563:HOH:O	2.11	0.51
1:B:237:ILE:HG12	1:B:331:ILE:CG1	2.41	0.51
1:B:186:VAL:O	1:B:189:PHE:HB2	2.11	0.50
1:A:34:LEU:HD13	1:A:144:TYR:HA	1.94	0.49
1:A:271:ASN:ND2	1:A:284:GLN:HB2	2.24	0.49
2:A:401:TLA:O4	2:A:401:TLA:O2	2.31	0.49
2:B:401:TLA:H2	3:B:402:GOL:H11	1.95	0.49
1:A:128:ALA:N	1:A:129:ARG:HB2	2.28	0.48
1:B:159:GLN:OE1	3:B:402:GOL:H2	2.14	0.48
1:B:68:ILE:HD11	1:B:84:LEU:HB3	1.96	0.48
1:B:173:VAL:HG22	1:B:174:PRO:HD3	1.95	0.48
1:B:50:PRO:O	1:B:51:GLY:O	2.32	0.48
1:A:293:LYS:HB2	1:A:294:PRO:CD	2.44	0.48
1:B:220:GLU:HA	1:B:221:PRO:HD2	1.77	0.47
1:A:275:GLY:C	1:A:276:ILE:HG13	2.34	0.47
1:B:134:ARG:HG2	1:B:335:MET:HE1	1.97	0.47
1:B:155:GLY:N	1:B:333:GLU:OE2	2.45	0.47
1:A:244:GLU:HB2	1:A:248:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLY:O	1:A:286:ILE:HA	2.15	0.47
1:B:7:GLY:HA3	1:B:10:PHE:O	2.15	0.47
1:B:331:ILE:HG13	1:B:331:ILE:O	2.14	0.46
1:B:160:ILE:O	1:B:161:GLY:C	2.51	0.46
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.44	0.46
1:A:7:GLY:O	1:A:11:ARG:HG3	2.15	0.46
1:A:210:LEU:HD21	1:A:287:ARG:HG3	1.97	0.46
1:A:248:GLY:O	1:A:251:VAL:HG22	2.15	0.46
1:A:238:ASN:O	1:A:239:ALA:CB	2.63	0.46
1:B:48:ARG:HH11	1:B:131:THR:HG22	1.81	0.46
1:A:244:GLU:HG2	1:A:289:ALA:HB3	1.98	0.46
1:A:51:GLY:CA	1:A:54:LYS:CB	2.89	0.46
1:B:237:ILE:HG12	1:B:331:ILE:HG12	1.98	0.45
1:A:173:VAL:HG22	1:A:174:PRO:HD3	1.98	0.45
1:B:326:VAL:H	1:B:326:VAL:HG22	1.43	0.45
1:A:89:ASP:OD2	1:A:90:GLN:NE2	2.50	0.45
1:A:319:ARG:C	1:A:320:HIS:CD2	2.90	0.45
1:A:329:THR:HB	1:A:330:PRO:HD3	1.99	0.45
1:B:60:LYS:HA	4:B:504:HOH:O	2.17	0.44
1:B:90:GLN:OE1	1:B:90:GLN:N	2.50	0.44
1:A:42:GLN:OE1	1:A:65:VAL:HG12	2.17	0.44
1:A:65:VAL:CG1	1:A:65:VAL:O	2.64	0.44
1:B:65:VAL:HA	1:B:85:ILE:HG12	1.99	0.44
1:B:191:ALA:O	1:B:195:SER:HB2	2.18	0.44
1:A:153:ILE:HA	1:A:210:LEU:O	2.18	0.43
1:A:350:GLN:HG3	1:B:1:MET:CE	2.48	0.43
1:B:284:GLN:H	1:B:284:GLN:HG2	1.47	0.43
1:B:284:GLN:HB3	4:B:544:HOH:O	2.19	0.43
1:A:167:LYS:HG2	1:A:168:LEU:N	2.33	0.43
1:B:166:GLU:HB3	4:B:532:HOH:O	2.18	0.43
1:B:68:ILE:N	1:B:68:ILE:HD12	2.33	0.43
1:A:2:ALA:HA	1:B:221:PRO:O	2.18	0.43
1:B:331:ILE:O	1:B:335:MET:HG2	2.19	0.43
1:A:269:LEU:HD23	1:A:269:LEU:N	2.34	0.42
1:A:319:ARG:HH11	1:A:319:ARG:HG3	1.84	0.42
1:B:170:TRP:HZ2	1:B:210:LEU:HD12	1.84	0.42
1:A:262:GLU:HB3	1:A:264:THR:H	1.85	0.42
1:B:6:ILE:HG22	1:B:12:VAL:HB	2.00	0.42
1:A:210:LEU:CD2	1:A:287:ARG:HG3	2.49	0.42
1:B:6:ILE:O	1:B:11:ARG:HA	2.20	0.42
1:A:37:THR:HG22	1:A:40:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLY:HA3	1:B:52:THR:HA	1.72	0.42
1:A:72:PHE:O	1:A:73:GLU:C	2.56	0.42
1:A:48:ARG:C	1:A:50:PRO:HD3	2.36	0.41
1:B:131:THR:HG23	1:B:131:THR:O	2.19	0.41
1:A:79:THR:O	1:A:80:PRO:C	2.58	0.41
1:A:151:VAL:HG23	1:A:213:LYS:O	2.19	0.41
1:B:225:ARG:HB3	1:B:227:ASP:OD1	2.20	0.41
1:B:258:GLU:N	1:B:258:GLU:OE1	2.53	0.41
1:B:218:TRP:CH2	1:B:344:PHE:HB2	2.55	0.41
1:A:148:LYS:HG2	1:A:149:PHE:CE2	2.56	0.41
1:B:56:ALA:O	1:B:57:THR:OG1	2.30	0.41
1:B:207:LEU:HD13	1:B:292:LEU:HD13	2.03	0.41
1:A:271:ASN:HD21	1:A:284:GLN:CB	2.24	0.41
1:B:11:ARG:O	1:B:27:VAL:HA	2.20	0.41
1:A:128:ALA:O	1:A:130:GLU:HG2	2.21	0.41
1:B:47:ARG:O	1:B:50:PRO:HD3	2.19	0.41
1:A:74:GLY:C	1:A:75:LYS:HG2	2.40	0.41
1:A:207:LEU:O	1:A:289:ALA:HA	2.21	0.41
1:B:38:GLU:HB2	4:B:514:HOH:O	2.20	0.40
1:B:210:LEU:HA	1:B:286:ILE:O	2.21	0.40
1:A:157:VAL:HG21	1:A:178:PHE:O	2.22	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	288/363 (79%)	273 (95%)	12 (4%)	3 (1%)	19	37
1	B	288/363 (79%)	271 (94%)	14 (5%)	3 (1%)	19	37
All	All	576/726 (79%)	544 (94%)	26 (4%)	6 (1%)	19	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	GLY
1	B	322	PRO
1	B	263	LEU
1	A	322	PRO
1	A	55	PHE
1	A	62	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	229/286 (80%)	211 (92%)	18 (8%)	15 29
1	B	229/286 (80%)	208 (91%)	21 (9%)	11 21
All	All	458/572 (80%)	419 (92%)	39 (8%)	13 25

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	48	ARG
1	A	88	THR
1	A	126	SER
1	A	129	ARG
1	A	154	ARG
1	A	163	GLU
1	A	206	LYS
1	A	227	ASP
1	A	258	GLU
1	A	260	ARG
1	A	262	GLU
1	A	263	LEU
1	A	265	SER
1	A	269	LEU
1	A	284	GLN
1	A	321	ASP

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Mol	Chain	Res	Type
1	A	331	ILE
1	B	1	MET
1	B	11	ARG
1	B	59	ARG
1	B	88	THR
1	B	90	GLN
1	B	129	ARG
1	B	131	THR
1	B	154	ARG
1	B	175	ASN
1	B	199	GLN
1	B	201	THR
1	B	245	ILE
1	B	251	VAL
1	B	265	SER
1	B	284	GLN
1	B	293	LYS
1	B	320	HIS
1	B	323	CYS
1	B	324	VAL
1	B	326	VAL
1	B	331	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	90	GLN
1	A	271	ASN
1	A	284	GLN
1	A	320	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	TLA	A	401	-	3,9,9	2.69	2 (66%)	6,12,12	1.79	3 (50%)
3	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.22	0
2	TLA	B	401	-	3,9,9	0.88	0	6,12,12	1.18	1 (16%)
3	GOL	B	402	-	5,5,5	0.48	0	5,5,5	0.37	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	TLA	A	401	-	-	0/4/12/12	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	TLA	B	401	-	-	0/4/12/12	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TLA	C3-C2	-2.76	1.44	1.53
2	A	401	TLA	O2-C2	3.38	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	TLA	O3-C3-C4	-2.32	105.36	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	TLA	C4-C3-C2	-2.30	108.64	113.35
2	A	401	TLA	O2-C2-C1	-2.24	105.55	111.21
2	A	401	TLA	O2-C2-C3	2.16	114.69	108.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TLA	2	0
2	B	401	TLA	1	0
3	B	402	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	294/363 (80%)	0.74	38 (12%)	5	3	11, 29, 61, 99	22 (7%)
1	B	294/363 (80%)	0.99	45 (15%)	3	1	12, 32, 80, 100	22 (7%)
All	All	588/726 (80%)	0.87	83 (14%)	4	2	11, 31, 70, 100	44 (7%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	GLN	15.5
1	B	56	ALA	13.2
1	B	261	ASP	13.0
1	B	53	SER	11.5
1	B	263	LEU	11.5
1	B	52	THR	10.4
1	A	56	ALA	10.0
1	B	51	GLY	9.8
1	A	54	LYS	9.8
1	A	55	PHE	9.7
1	B	260	ARG	9.6
1	B	55	PHE	9.4
1	B	262	GLU	9.3
1	A	53	SER	9.2
1	A	268	PHE	8.7
1	A	260	ARG	8.6
1	A	265	SER	8.6
1	B	57	THR	8.4
1	A	52	THR	8.3
1	A	259	THR	8.3
1	B	257	HIS	7.9
1	A	263	LEU	7.8
1	B	259	THR	7.6
1	A	257	HIS	7.4

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Mol	Chain	Res	Type	RSRZ
1	B	59	ARG	7.2
1	B	54	LYS	7.0
1	A	59	ARG	6.8
1	A	127	SER	6.6
1	A	264	THR	6.5
1	B	258	GLU	6.4
1	B	318	GLY	6.4
1	A	261	ASP	6.1
1	A	90	GLN	6.0
1	B	321	ASP	5.8
1	B	126	SER	5.6
1	A	267	GLY	5.6
1	A	57	THR	5.5
1	B	319	ARG	5.4
1	A	51	GLY	5.4
1	A	319	ARG	5.3
1	B	268	PHE	5.1
1	A	58	GLN	5.1
1	A	184	ASP	5.0
1	A	50	PRO	5.0
1	A	256	GLY	4.8
1	B	320	HIS	4.4
1	B	197	ARG	4.4
1	A	126	SER	4.3
1	B	201	THR	4.3
1	A	49	LYS	4.2
1	B	50	PRO	4.2
1	A	89	ASP	4.1
1	B	265	SER	4.1
1	B	267	GLY	4.0
1	A	258	GLU	4.0
1	B	49	LYS	3.9
1	A	318	GLY	3.7
1	B	200	GLY	3.7
1	B	269	LEU	3.7
1	B	264	THR	3.4
1	B	127	SER	3.4
1	A	175	ASN	3.2
1	B	60	LYS	3.0
1	A	266	HIS	3.0
1	B	90	GLN	2.7
1	B	327	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	2.7
1	A	61	GLU	2.6
1	A	167	LYS	2.6
1	B	266	HIS	2.6
1	B	198	GLU	2.5
1	A	255	PHE	2.5
1	B	256	GLY	2.4
1	A	185	ALA	2.2
1	B	199	GLN	2.2
1	B	272	HIS	2.2
1	B	61	GLU	2.2
1	A	269	LEU	2.1
1	A	164	VAL	2.1
1	B	190	GLU	2.1
1	B	89	ASP	2.0
1	B	88	THR	2.0
1	B	270	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	402	6/6	0.44	0.40	3.69	64,73,75,79	0
2	TLA	B	401	10/10	0.57	0.45	-	89,90,91,93	0
2	TLA	A	401	10/10	0.60	0.47	-	80,81,81,81	0
3	GOL	A	402	6/6	0.51	0.46	-	77,77,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.