



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 AM GMT

PDB ID : 2Y0E
Title : BCEC AND THE FINAL STEP OF UGDS REACTION
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Deposited on : 2010-12-02
Resolution : 1.75 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

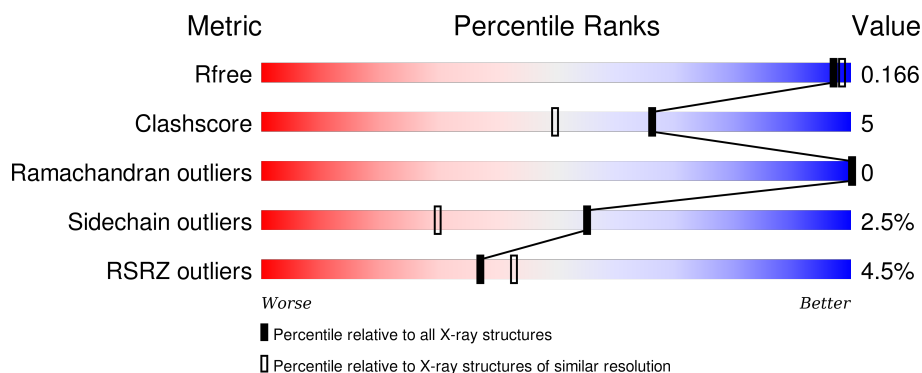
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 $\leq 5\%$. 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	478	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
1	B	478	<div> <div>3%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	C	478	<div> <div>9%</div> <div>86%</div> <div>9%</div> <div>• 5%</div> </div>
1	D	478	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>

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	SO4	A	1460	-	-	-	X
3	SO4	A	1462	-	-	-	X
3	SO4	B	1461	-	-	-	X
3	SO4	B	1462	-	-	-	X
3	SO4	C	1459	-	-	-	X
3	SO4	D	1460	-	-	-	X
4	ACT	B	1463	-	-	-	X
5	GOL	A	1465	-	-	-	X
5	GOL	A	1466	-	-	X	-
5	GOL	C	1463	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16024 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 UDP-GLUCOSE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	19	0
			3624	2277	645	687	15			
1	B	451	Total	C	N	O	S	0	22	0
			3578	2248	643	672	15			
1	C	455	Total	C	N	O	S	0	14	0
			3563	2238	632	678	15			
1	D	454	Total	C	N	O	S	0	30	0
			3616	2262	657	679	18			

There are 32 discrepancies between the modelled and reference sequences:

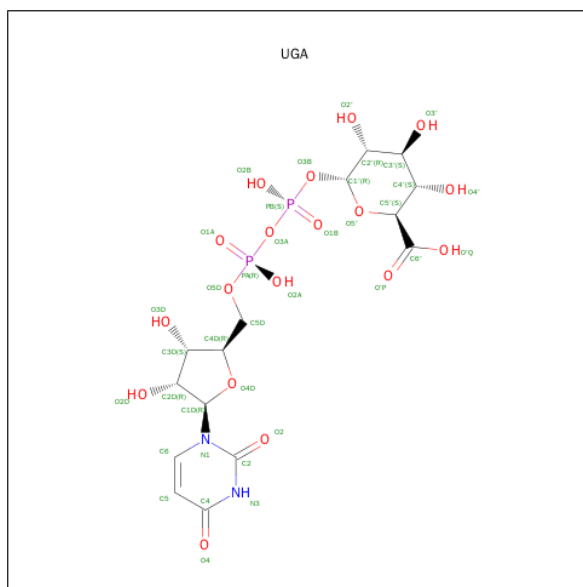
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP C9E261
A	-7	HIS	-	EXPRESSION TAG	UNP C9E261
A	-6	HIS	-	EXPRESSION TAG	UNP C9E261
A	-5	HIS	-	EXPRESSION TAG	UNP C9E261
A	-4	HIS	-	EXPRESSION TAG	UNP C9E261
A	-3	HIS	-	EXPRESSION TAG	UNP C9E261
A	-2	GLY	-	EXPRESSION TAG	UNP C9E261
A	-1	SER	-	EXPRESSION TAG	UNP C9E261
B	-8	HIS	-	EXPRESSION TAG	UNP C9E261
B	-7	HIS	-	EXPRESSION TAG	UNP C9E261
B	-6	HIS	-	EXPRESSION TAG	UNP C9E261
B	-5	HIS	-	EXPRESSION TAG	UNP C9E261
B	-4	HIS	-	EXPRESSION TAG	UNP C9E261
B	-3	HIS	-	EXPRESSION TAG	UNP C9E261
B	-2	GLY	-	EXPRESSION TAG	UNP C9E261
B	-1	SER	-	EXPRESSION TAG	UNP C9E261
C	-8	HIS	-	EXPRESSION TAG	UNP C9E261
C	-7	HIS	-	EXPRESSION TAG	UNP C9E261
C	-6	HIS	-	EXPRESSION TAG	UNP C9E261
C	-5	HIS	-	EXPRESSION TAG	UNP C9E261
C	-4	HIS	-	EXPRESSION TAG	UNP C9E261

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	EXPRESSION TAG	UNP C9E261
C	-2	GLY	-	EXPRESSION TAG	UNP C9E261
C	-1	SER	-	EXPRESSION TAG	UNP C9E261
D	-8	HIS	-	EXPRESSION TAG	UNP C9E261
D	-7	HIS	-	EXPRESSION TAG	UNP C9E261
D	-6	HIS	-	EXPRESSION TAG	UNP C9E261
D	-5	HIS	-	EXPRESSION TAG	UNP C9E261
D	-4	HIS	-	EXPRESSION TAG	UNP C9E261
D	-3	HIS	-	EXPRESSION TAG	UNP C9E261
D	-2	GLY	-	EXPRESSION TAG	UNP C9E261
D	-1	SER	-	EXPRESSION TAG	UNP C9E261

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$).



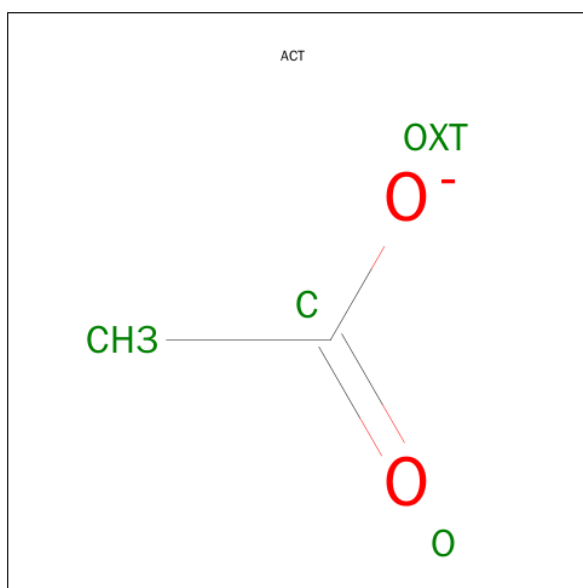
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
2	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



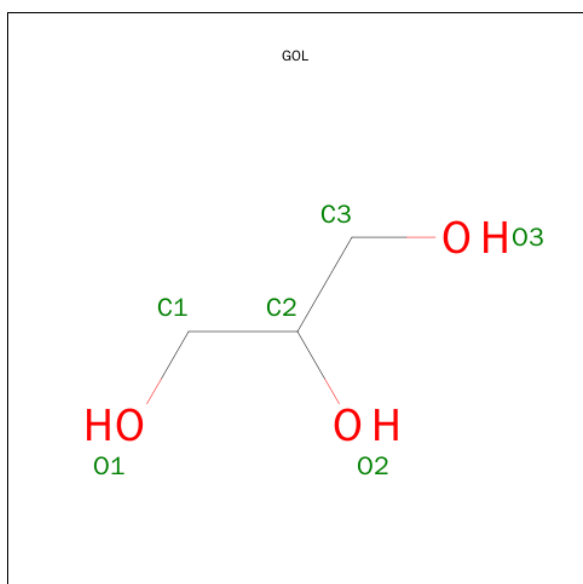
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

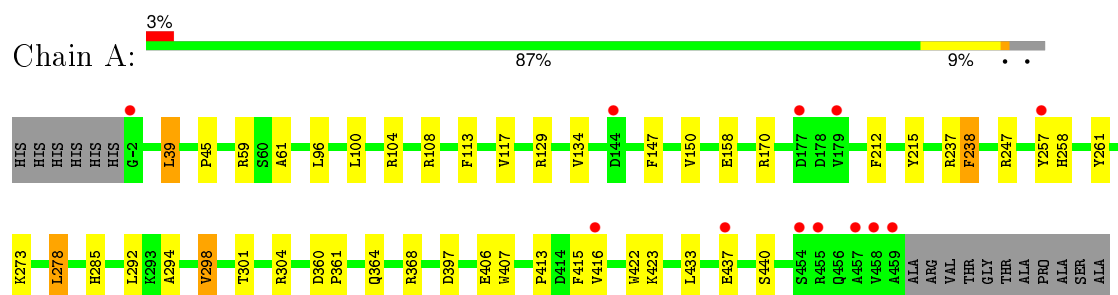
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	380	Total O 380 380	0	0
6	B	330	Total O 330 330	0	0
6	C	289	Total O 289 289	0	0
6	D	374	Total O 374 374	0	0

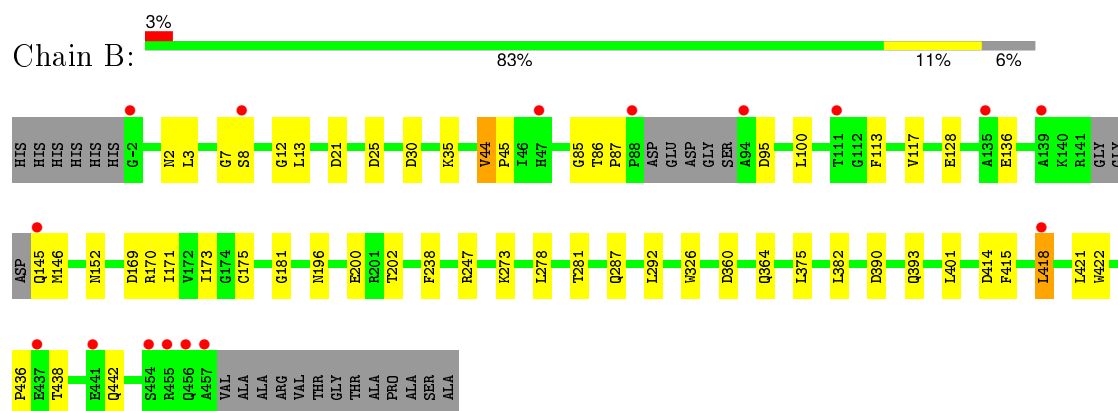
3 Residue-property plots

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.

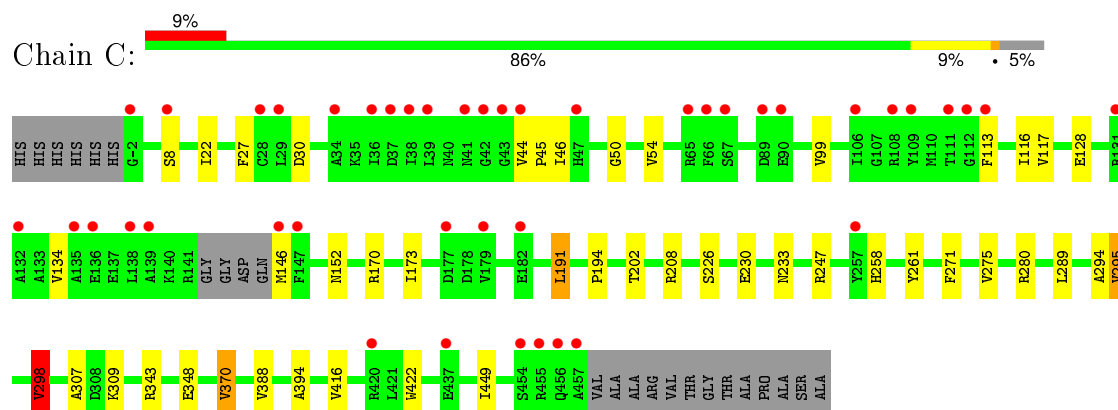
• Molecule 1: UDP-GLUCOSE DEHYDROGENASE



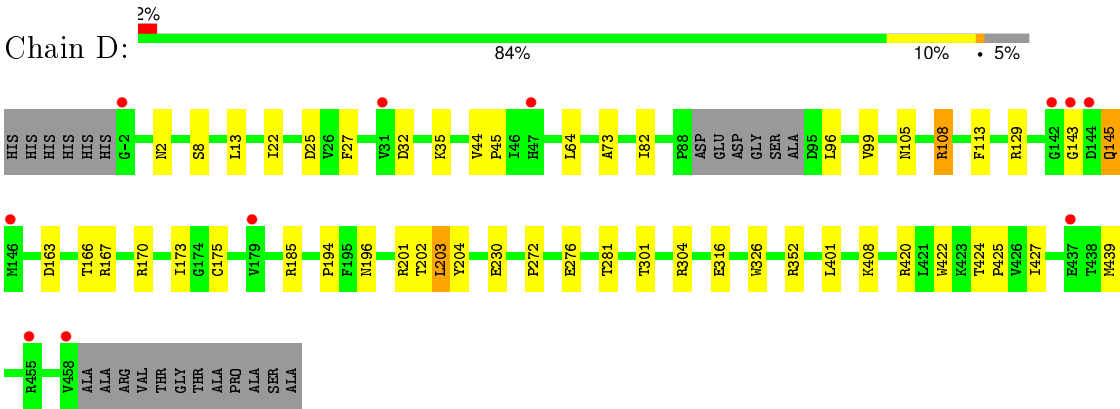
• Molecule 1: UDP-GLUCOSE DEHYDROGENASE



• Molecule 1: UDP-GLUCOSE DEHYDROGENASE



• Molecule 1: UDP-GLUCOSE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.63Å 108.93Å 187.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.69 – 1.75 47.42 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (35.69-1.75) 98.2 (47.42-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.197 0.164 , 0.166	Depositor DCC
R_{free} test set	9969 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 197642 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16024	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, UGA, SO4, ACT

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	0.58	0/3784	0.67	0/5123
1	B	0.56	0/3740	0.68	1/5062 (0.0%)
1	C	0.55	0/3693	0.66	1/5000 (0.0%)
1	D	0.58	0/3842	0.68	0/5192
All	All	0.57	0/15059	0.67	2/20377 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	LEU	CA-CB-CG	8.57	135.00	115.30
1	C	298	VAL	CG1-CB-CG2	5.75	120.10	110.90

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	3624	0	3595	34	0
1	B	3578	0	3552	45	0
1	C	3563	0	3523	29	0
1	D	3616	0	3572	41	0
2	A	37	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	0	19	0	0
2	C	37	0	19	0	0
2	D	37	0	19	0	0
3	A	15	0	0	0	0
3	B	25	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	A	18	0	24	6	0
5	C	12	0	16	4	0
5	D	6	0	8	3	0
6	A	380	0	0	5	0
6	B	330	0	0	4	0
6	C	289	0	0	6	0
6	D	374	0	0	3	0
All	All	16024	0	14378	144	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 5.

All (144) 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:59[B]:ARG:HD2	6:A:2068:HOH:O	1.72	0.88
1:D:427:ILE:HD12	1:D:439[B]:MET:HE1	1.57	0.85
1:A:258:HIS:HA	5:A:1466:GOL:H32	1.63	0.81
1:A:360:ASP:H	1:A:364[B]:GLN:HE21	1.29	0.79
1:D:113:PHE:H	5:D:1463:GOL:H31	1.50	0.77
1:D:143:GLY:HA3	1:D:145[A]:GLN:HE22	1.50	0.76
1:A:261:TYR:CE2	5:A:1466:GOL:H31	2.22	0.75
1:A:261:TYR:HE2	5:A:1466:GOL:H31	1.55	0.72
1:B:390:ASP:CG	1:B:393[B]:GLN:HE21	1.93	0.72
1:B:86[A]:THR:O	1:B:273:LYS:HD2	1.90	0.71
1:B:360:ASP:H	1:B:364[A]:GLN:HE21	1.39	0.69
1:A:397:ASP:O	1:A:423[A]:LYS:HE3	1.93	0.69
1:D:316[B]:GLU:HG3	1:D:352:ARG:HH12	1.58	0.68
1:C:307:ALA:HB1	1:C:348[B]:GLU:HG2	1.75	0.68
1:B:8:SER:HB3	1:B:13[B]:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87[B]:PRO:O	1:B:95:ASP:HB3	1.94	0.66
1:D:105:ASN:HA	1:D:108[B]:ARG:HG2	1.76	0.66
1:A:301:THR:HG22	1:A:304:ARG:NH2	2.11	0.65
1:C:307:ALA:CB	1:C:348[B]:GLU:HG2	2.27	0.65
1:D:196:ASN:ND2	1:D:201:ARG:H	1.95	0.65
1:D:230[B]:GLU:HG3	6:D:2206:HOH:O	1.97	0.64
1:C:247:ARG:NH2	6:C:2125:HOH:O	2.32	0.61
1:A:134:VAL:HG22	1:A:147:PHE:CZ	2.35	0.61
5:C:1463:GOL:H32	6:C:2265:HOH:O	1.99	0.61
1:C:22:ILE:HD12	1:C:194:PRO:HG2	1.83	0.60
1:D:32:ASP:OD2	1:D:35:LYS:HE3	2.02	0.60
1:C:233[A]:ASN:ND2	6:C:2116:HOH:O	2.35	0.59
1:C:271:PHE:O	1:C:275:VAL:HG13	2.02	0.59
1:D:96:LEU:HD22	1:D:129[B]:ARG:NH1	2.18	0.59
1:C:8:SER:OG	1:C:30:ASP:HB2	2.03	0.58
1:D:301[B]:THR:HG22	1:D:304:ARG:NH2	2.19	0.58
1:A:39:LEU:HD13	1:A:45[A]:PRO:HD3	1.86	0.57
1:D:143:GLY:HA3	1:D:145[A]:GLN:NE2	2.18	0.57
1:C:230:GLU:HG3	1:C:298:VAL:HG11	1.88	0.56
1:D:420[A]:ARG:HH11	1:D:420[A]:ARG:HG2	1.70	0.56
1:D:316[B]:GLU:HG3	1:D:352:ARG:NH1	2.21	0.55
1:B:414:ASP:O	1:B:418:LEU:HD23	2.06	0.55
1:B:8:SER:HB3	1:B:13[B]:LEU:CD2	2.37	0.55
1:D:113:PHE:N	5:D:1463:GOL:H31	2.21	0.55
1:A:247:ARG:NH2	6:A:2232:HOH:O	2.39	0.55
1:A:285:HIS:NE2	5:A:1465:GOL:H2	2.23	0.54
1:B:200:GLU:OE2	1:B:202[B]:THR:OG1	2.23	0.54
1:B:173[A]:ILE:HD12	1:B:202[A]:THR:HG21	1.89	0.54
1:B:8:SER:HB2	1:B:35:LYS:NZ	2.24	0.53
1:D:272:PRO:O	1:D:276[B]:GLU:HG2	2.09	0.53
1:A:237:ARG:HD2	1:B:287:GLN:HE21	1.72	0.53
1:B:438:THR:O	1:B:442:GLN:HG3	2.08	0.53
1:A:215:TYR:HB3	1:A:278:LEU:HG	1.90	0.52
1:B:169:ASP:HB2	6:B:2123:HOH:O	2.08	0.52
1:D:175[B]:CYS:SG	1:D:185[B]:ARG:HG3	2.50	0.52
1:B:196:ASN:HD21	1:B:202[B]:THR:HG23	1.75	0.51
1:B:173[A]:ILE:HD12	1:B:202[A]:THR:CG2	2.40	0.51
1:B:171:ILE:HB	1:B:202[B]:THR:HG22	1.92	0.51
1:D:173:ILE:HD12	1:D:202[B]:THR:CG2	2.40	0.51
1:A:96:LEU:HD12	1:A:129:ARG:NH1	2.25	0.51
1:D:173:ILE:HD12	1:D:202[B]:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59[B]:ARG:NH2	6:A:2059:HOH:O	2.43	0.50
1:D:2:ASN:HD22	1:D:25:ASP:HB3	1.76	0.50
1:B:86[B]:THR:HG22	6:B:2062:HOH:O	2.12	0.50
1:B:2:ASN:HD22	1:B:25:ASP:HB3	1.75	0.50
1:A:158:GLU:HB2	6:A:2013:HOH:O	2.12	0.50
1:D:301[B]:THR:HG22	1:D:304:ARG:HH22	1.76	0.50
1:A:117:VAL:HG22	1:A:150[B]:VAL:CG2	2.42	0.50
1:A:437:GLU:O	1:A:440:SER:HB2	2.12	0.50
1:B:86[B]:THR:HB	1:B:95:ASP:O	2.12	0.49
1:C:50:GLY:O	1:C:54:VAL:HG23	2.12	0.49
1:B:21:ASP:OD2	1:D:408:LYS:HE2	2.11	0.49
1:A:258:HIS:ND1	5:A:1466:GOL:H12	2.28	0.49
1:C:173:ILE:HD12	1:C:202:THR:HG21	1.95	0.49
1:D:163:ASP:HA	1:D:166[B]:THR:HG22	1.94	0.48
1:C:294:ALA:O	1:C:298:VAL:HG13	2.13	0.48
1:D:202[B]:THR:HG21	1:D:204:TYR:CZ	2.48	0.48
1:D:427:ILE:HD12	1:D:439[B]:MET:CE	2.38	0.48
1:B:390:ASP:OD1	1:B:393[B]:GLN:HG3	2.14	0.48
1:B:87[B]:PRO:O	1:B:95:ASP:CB	2.62	0.48
1:C:343:ARG:CZ	1:C:370:VAL:HG13	2.44	0.48
1:D:203[A]:LEU:HD22	6:D:2194:HOH:O	2.13	0.47
1:C:388:VAL:HG21	1:C:394:ALA:HB2	1.97	0.47
1:B:375:LEU:HB2	1:B:382:LEU:HD21	1.97	0.47
1:C:226:SER:HB2	1:C:295:VAL:HB	1.96	0.47
1:A:294:ALA:O	1:A:298:VAL:HG13	2.15	0.47
1:C:261:TYR:HE2	5:C:1462:GOL:H2	1.80	0.47
1:D:22:ILE:HD12	1:D:194:PRO:HG2	1.97	0.47
1:D:96:LEU:HD12	1:D:96:LEU:N	2.31	0.46
1:C:116:ILE:HD13	1:C:134:VAL:HG21	1.97	0.46
1:A:104[A]:ARG:NH2	6:A:2113:HOH:O	2.44	0.46
1:A:113:PHE:HB2	5:A:1464:GOL:H2	1.97	0.45
1:B:175[B]:CYS:SG	1:B:181:GLY:O	2.75	0.45
1:B:415:PHE:HA	1:B:418:LEU:HD23	1.98	0.45
1:B:113:PHE:HA	1:B:146:MET:O	2.17	0.45
1:B:8:SER:HB2	1:B:35:LYS:CE	2.47	0.45
1:C:289:LEU:HD22	1:D:230[B]:GLU:HG2	1.99	0.45
1:B:128:GLU:HG3	6:B:2145:HOH:O	2.15	0.45
5:C:1463:GOL:C3	6:C:2265:HOH:O	2.62	0.44
1:B:7:GLY:HA2	1:B:30:ASP:OD1	2.18	0.44
1:C:191:LEU:HD12	1:C:191:LEU:O	2.17	0.44
1:D:44:VAL:HA	1:D:45:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247[B]:ARG:NE	6:B:2163:HOH:O	2.49	0.43
1:A:237:ARG:HH11	1:B:287:GLN:NE2	2.17	0.43
1:A:292:LEU:HA	1:A:292:LEU:HD23	1.86	0.43
1:A:238[B]:PHE:CZ	1:B:281:THR:CG2	3.01	0.43
1:A:238[B]:PHE:CZ	1:B:281:THR:HG22	2.53	0.43
1:C:230:GLU:CG	1:C:298:VAL:HG11	2.50	0.42
1:A:61:ALA:HA	1:C:416:VAL:HG21	2.01	0.42
1:C:117:VAL:CG1	1:C:152:ASN:HB3	2.49	0.42
1:B:44:VAL:HA	1:B:45[B]:PRO:HD3	1.61	0.42
1:B:8:SER:HB2	1:B:35:LYS:HZ1	1.83	0.42
1:C:309:LYS:HE3	1:C:449:ILE:HD13	2.01	0.42
1:A:257[B]:TYR:CE1	1:A:258:HIS:CE1	3.08	0.42
1:C:128[B]:GLU:CD	1:C:208:ARG:HH21	2.23	0.42
1:A:361:PRO:HG2	1:A:407:TRP:CD2	2.55	0.42
1:D:196:ASN:HD22	1:D:201:ARG:H	1.64	0.42
1:C:233[B]:ASN:ND2	6:C:2118:HOH:O	2.52	0.42
1:B:8:SER:HB2	1:B:35:LYS:HE3	2.02	0.41
1:B:8:SER:C	1:B:35:LYS:HZ2	2.23	0.41
1:B:7:GLY:O	1:B:12:GLY:HA3	2.20	0.41
1:B:86[B]:THR:N	1:B:87[B]:PRO:HD3	2.35	0.41
1:D:326:TRP:CG	1:D:401:LEU:HD11	2.55	0.41
1:C:44:VAL:HG12	1:C:46:ILE:H	1.86	0.41
1:A:117:VAL:HG22	1:A:150[B]:VAL:HG21	2.03	0.41
1:D:281[B]:THR:HG21	6:D:2116:HOH:O	2.20	0.41
1:B:292:LEU:HA	1:B:292:LEU:HD23	1.81	0.41
1:C:128[B]:GLU:HG3	6:C:2051:HOH:O	2.21	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.78	0.41
1:D:82:ILE:HG21	1:D:99:VAL:HB	2.03	0.41
1:D:8:SER:O	1:D:13:LEU:HG	2.21	0.41
1:B:117:VAL:CG1	1:B:152:ASN:HB3	2.50	0.41
1:C:113:PHE:HA	1:C:146:MET:O	2.21	0.41
1:B:390:ASP:N	1:B:393[B]:GLN:NE2	2.69	0.41
1:B:85[A]:GLY:C	1:B:87[A]:PRO:HD3	2.42	0.41
1:A:100:LEU:O	1:A:104[B]:ARG:HG3	2.21	0.41
1:D:27:PHE:CE1	1:D:73:ALA:HB2	2.56	0.41
1:D:424:THR:HA	1:D:425[A]:PRO:HD3	1.89	0.41
1:D:113:PHE:H	5:D:1463:GOL:C3	2.25	0.40
1:B:326:TRP:CG	1:B:401:LEU:HD11	2.56	0.40
1:A:406:GLU:HB2	1:A:433:LEU:HD21	2.02	0.40
1:C:258:HIS:ND1	5:C:1462:GOL:H12	2.37	0.40
1:A:413:PRO:HG2	1:A:415:PHE:CE2	2.57	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	479/478 (100%)	474 (99%)	5 (1%)	0	100	100
1	B	467/478 (98%)	456 (98%)	11 (2%)	0	100	100
1	C	465/478 (97%)	461 (99%)	4 (1%)	0	100	100
1	D	481/478 (101%)	471 (98%)	10 (2%)	0	100	100
All	All	1892/1912 (99%)	1862 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	385/377 (102%)	374 (97%)	11 (3%)	50	24
1	B	381/377 (101%)	371 (97%)	10 (3%)	54	28
1	C	376/377 (100%)	367 (98%)	9 (2%)	57	31
1	D	392/377 (104%)	382 (97%)	10 (3%)	54	28
All	All	1534/1508 (102%)	1494 (97%)	40 (3%)	55	28

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	108	ARG
1	A	170	ARG
1	A	212	PHE
1	A	238[A]	PHE
1	A	238[B]	PHE
1	A	273	LYS
1	A	278	LEU
1	A	298	VAL
1	A	416	VAL
1	A	422	TRP
1	B	3	LEU
1	B	44	VAL
1	B	100	LEU
1	B	136	GLU
1	B	145	GLN
1	B	170	ARG
1	B	238	PHE
1	B	278	LEU
1	B	421	LEU
1	B	422	TRP
1	C	27	PHE
1	C	99	VAL
1	C	170	ARG
1	C	191	LEU
1	C	280	ARG
1	C	295	VAL
1	C	298	VAL
1	C	370	VAL
1	C	422	TRP
1	D	64	LEU
1	D	108[A]	ARG
1	D	108[B]	ARG
1	D	145[A]	GLN
1	D	145[B]	GLN
1	D	167	ARG
1	D	170	ARG
1	D	203[A]	LEU
1	D	203[B]	LEU
1	D	422	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	152	ASN
1	A	287	GLN
1	B	2	ASN
1	B	33	GLN
1	B	40	ASN
1	B	287	GLN
1	B	333	ASN
1	C	40	ASN
1	C	97	GLN
1	C	105	ASN
1	D	2	ASN
1	D	33	GLN
1	D	40	ASN
1	D	97	GLN
1	D	196	ASN
1	D	233	ASN
1	D	442	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

28 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
3	SO4	A	1460	-	4,4,4	0.12	0	6,6,6	0.42	0
3	SO4	A	1461	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	A	1462	-	4,4,4	0.22	0	6,6,6	0.11	0
4	ACT	A	1463	-	1,3,3	0.36	0	0,3,3	0.00	-
5	GOL	A	1464	-	5,5,5	0.20	0	5,5,5	0.27	0
5	GOL	A	1465	-	5,5,5	0.27	0	5,5,5	0.47	0
5	GOL	A	1466	-	5,5,5	0.17	0	5,5,5	0.59	0
2	UGA	A	501	-	27,39,39	0.74	0	41,60,60	1.55	8 (19%)
3	SO4	B	1458	-	4,4,4	0.45	0	6,6,6	0.16	0
3	SO4	B	1459	-	4,4,4	0.26	0	6,6,6	0.40	0
3	SO4	B	1460	-	4,4,4	0.19	0	6,6,6	0.10	0
3	SO4	B	1461	-	4,4,4	0.19	0	6,6,6	0.12	0
3	SO4	B	1462	-	4,4,4	0.18	0	6,6,6	0.21	0
4	ACT	B	1463	-	1,3,3	0.56	0	0,3,3	0.00	-
2	UGA	B	501	-	27,39,39	0.78	1 (3%)	41,60,60	1.36	3 (7%)
3	SO4	C	1458	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	C	1459	-	4,4,4	0.13	0	6,6,6	0.29	0
3	SO4	C	1460	-	4,4,4	0.18	0	6,6,6	0.19	0
4	ACT	C	1461	-	1,3,3	1.24	0	0,3,3	0.00	-
5	GOL	C	1462	-	5,5,5	0.33	0	5,5,5	0.46	0
5	GOL	C	1463	-	5,5,5	0.31	0	5,5,5	0.33	0
2	UGA	C	501	-	27,39,39	0.62	0	41,60,60	1.26	3 (7%)
3	SO4	D	1459	-	4,4,4	0.16	0	6,6,6	0.33	0
3	SO4	D	1460	-	4,4,4	0.11	0	6,6,6	0.22	0
3	SO4	D	1461	-	4,4,4	0.19	0	6,6,6	0.11	0
4	ACT	D	1462	-	1,3,3	0.41	0	0,3,3	0.00	-
5	GOL	D	1463	-	5,5,5	0.20	0	5,5,5	0.36	0
2	UGA	D	501	-	27,39,39	0.78	0	41,60,60	1.53	5 (12%)

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
3	SO4	A	1460	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1461	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1462	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1463	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1464	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1465	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1466	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UGA	A	501	-	-	0/17/61/61	0/3/3/3
3	SO4	B	1458	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1459	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1460	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1461	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1462	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1463	-	-	0/0/0/0	0/0/0/0
2	UGA	B	501	-	-	0/17/61/61	0/3/3/3
3	SO4	C	1458	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1459	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1460	-	-	0/0/0/0	0/0/0/0
4	ACT	C	1461	-	-	0/0/0/0	0/0/0/0
5	GOL	C	1462	-	-	0/4/4/4	0/0/0/0
5	GOL	C	1463	-	-	0/4/4/4	0/0/0/0
2	UGA	C	501	-	-	0/17/61/61	0/3/3/3
3	SO4	D	1459	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1460	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1461	-	-	0/0/0/0	0/0/0/0
4	ACT	D	1462	-	-	0/0/0/0	0/0/0/0
5	GOL	D	1463	-	-	0/4/4/4	0/0/0/0
2	UGA	D	501	-	-	0/17/61/61	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UGA	O4D-C1D	2.75	1.44	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	UGA	C6'-C5'-C4'	-3.11	104.23	113.00
2	B	501	UGA	C6'-C5'-C4'	-3.04	104.41	113.00
2	D	501	UGA	C6'-C5'-C4'	-2.97	104.61	113.00
2	D	501	UGA	O5'-C1'-C2'	-2.67	104.81	110.28
2	A	501	UGA	O3D-C3D-C4D	-2.45	103.71	111.05
2	A	501	UGA	C4'-C3'-C2'	-2.20	106.69	110.79
2	A	501	UGA	C6'-C5'-C4'	-2.13	106.98	113.00
2	A	501	UGA	O2'-C2'-C3'	-2.05	105.73	110.34
2	D	501	UGA	O3B-PB-O1B	-2.00	101.58	109.46
2	A	501	UGA	C1'-O5'-C5'	2.12	115.45	112.17
2	A	501	UGA	O2B-PB-O1B	2.34	125.23	112.53
2	C	501	UGA	C1'-O5'-C5'	2.64	116.26	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UGA	C1'-O5'-C5'	2.78	116.49	112.17
2	D	501	UGA	C1'-O5'-C5'	2.83	116.56	112.17
2	A	501	UGA	PA-O3A-PB	3.22	141.78	132.73
2	C	501	UGA	C4-N3-C2	4.68	118.77	114.14
2	B	501	UGA	C4-N3-C2	5.75	119.84	114.14
2	A	501	UGA	C4-N3-C2	6.07	120.15	114.14
2	D	501	UGA	C4-N3-C2	6.32	120.40	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1464	GOL	1	0
5	A	1465	GOL	1	0
5	A	1466	GOL	4	0
5	C	1462	GOL	2	0
5	C	1463	GOL	2	0
5	D	1463	GOL	3	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	461/478 (96%)	-0.08	12 (2%) 59 65	9, 19, 36, 68	0
1	B	451/478 (94%)	0.03	16 (3%) 48 53	8, 20, 45, 66	0
1	C	455/478 (95%)	0.39	43 (9%) 10 13	8, 24, 63, 91	0
1	D	454/478 (94%)	-0.03	11 (2%) 62 69	7, 19, 40, 75	0
All	All	1821/1912 (95%)	0.08	82 (4%) 37 43	7, 20, 47, 91	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	143	GLY	5.3
1	B	94	ALA	5.2
1	C	38	ILE	5.2
1	C	139	ALA	4.9
1	C	44	VAL	4.7
1	C	257[A]	TYR	4.6
1	A	455	ARG	4.5
1	A	257[A]	TYR	4.5
1	B	455	ARG	4.4
1	C	113	PHE	4.3
1	C	455	ARG	4.1
1	A	144	ASP	4.0
1	C	112	GLY	3.9
1	B	47	HIS	3.8
1	C	146	MET	3.7
1	D	31	VAL	3.7
1	A	459	ALA	3.6
1	A	458	VAL	3.5
1	C	39	LEU	3.5
1	B	457	ALA	3.5
1	C	147	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	ALA	3.4
1	B	88[A]	PRO	3.3
1	C	29	LEU	3.3
1	C	34	ALA	3.3
1	D	455[A]	ARG	3.2
1	C	131	ARG	3.1
1	C	138	LEU	3.0
1	B	-2	GLY	3.0
1	C	111	THR	3.0
1	D	144	ASP	3.0
1	B	454	SER	3.0
1	A	416	VAL	2.9
1	C	182	GLU	2.9
1	B	135	ALA	2.8
1	C	65	ARG	2.8
1	B	456	GLN	2.8
1	C	42	GLY	2.7
1	C	36	ILE	2.7
1	C	8	SER	2.7
1	C	41	ASN	2.7
1	D	146[A]	MET	2.6
1	C	-2	GLY	2.6
1	A	-2	GLY	2.6
1	D	-2	GLY	2.6
1	B	418	LEU	2.6
1	C	454	SER	2.5
1	C	37	ASP	2.5
1	B	145	GLN	2.5
1	A	457	ALA	2.4
1	D	437	GLU	2.4
1	D	142	GLY	2.4
1	C	177	ASP	2.4
1	C	135	ALA	2.4
1	C	67	SER	2.4
1	C	136	GLU	2.4
1	C	89	ASP	2.4
1	C	456	GLN	2.4
1	B	441	GLU	2.3
1	C	47	HIS	2.3
1	C	109	TYR	2.3
1	A	179	VAL	2.3
1	C	420	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	458	VAL	2.3
1	C	90	GLU	2.3
1	C	108	ARG	2.3
1	A	177	ASP	2.3
1	C	132	ALA	2.3
1	A	454	SER	2.3
1	C	66	PHE	2.3
1	C	28[A]	CYS	2.3
1	C	106	ILE	2.2
1	C	179	VAL	2.2
1	B	437	GLU	2.2
1	C	437	GLU	2.2
1	D	179	VAL	2.2
1	D	47	HIS	2.1
1	C	43	GLY	2.1
1	B	111	THR	2.1
1	B	8	SER	2.1
1	A	437	GLU	2.1
1	C	457	ALA	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	D	1460	5/5	0.87	0.22	16.94	69,71,71,72	0
3	SO4	C	1459	5/5	0.88	0.28	12.06	41,53,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	B	1462	5/5	0.86	0.18	5.55	73,75,75,76	0
5	GOL	C	1463	6/6	0.79	0.18	5.48	46,55,57,57	0
5	GOL	A	1465	6/6	0.79	0.14	4.22	57,58,60,60	0
3	SO4	A	1462	5/5	0.86	0.23	3.58	88,89,89,89	0
3	SO4	B	1461	5/5	0.82	0.21	2.34	93,94,94,95	0
3	SO4	A	1460	5/5	0.96	0.12	2.28	44,48,51,51	0
4	ACT	B	1463	4/4	0.93	0.17	2.05	23,24,25,29	0
4	ACT	C	1461	4/4	0.97	0.11	1.73	26,26,26,29	0
3	SO4	D	1461	5/5	0.85	0.28	1.07	93,94,94,94	0
4	ACT	D	1462	4/4	0.95	0.10	0.61	23,24,24,28	0
5	GOL	A	1466	6/6	0.91	0.18	0.32	21,40,47,49	0
4	ACT	A	1463	4/4	0.98	0.08	-0.12	16,18,20,21	0
3	SO4	B	1459	5/5	0.95	0.11	-0.35	31,38,39,45	0
2	UGA	A	501	37/37	0.98	0.08	-0.42	7,11,16,21	0
3	SO4	B	1458	5/5	0.99	0.07	-0.49	19,22,25,26	0
5	GOL	C	1462	6/6	0.94	0.14	-0.52	18,37,42,47	0
2	UGA	B	501	37/37	0.99	0.09	-0.53	7,10,14,17	0
2	UGA	C	501	37/37	0.99	0.08	-0.60	8,11,17,19	0
2	UGA	D	501	37/37	0.99	0.08	-0.94	6,10,15,20	0
3	SO4	B	1460	5/5	0.91	0.19	-	72,72,73,75	0
3	SO4	A	1461	5/5	0.94	0.11	-	59,60,63,65	0
3	SO4	C	1460	5/5	0.84	0.28	-	87,87,88,89	0
5	GOL	A	1464	6/6	0.90	0.23	-	44,46,48,48	0
3	SO4	D	1459	5/5	0.95	0.10	-	32,38,40,41	0
5	GOL	D	1463	6/6	0.91	0.16	-	41,44,47,50	0
3	SO4	C	1458	5/5	0.97	0.11	-	44,45,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.