Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:55 AM EDT

PDB ID	:	1X0V
Title	:	Crystal Structure of Homo Sapien Glycerol-3-Phosphate Dehydrogenase 1
Authors	:	Rao, Z.; Ou, X.
Deposited on	:	2005-03-30
Resolution	:	2.30 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:

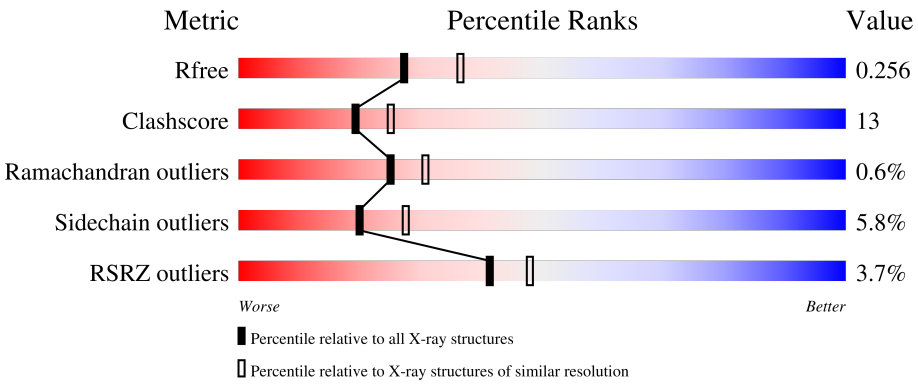
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	354	3% 72% 22%
1	B	354	4% 76% 20%

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
2	SO4	A	1002	-	-	-	X
2	SO4	B	1010	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5977 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 Glycerol-3-phosphate dehydrogenase [NAD+], cytoplasmic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	348	2624	1670	445	490	11	8	0	0	0
1	B	349	2632	1675	446	491	11	9	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

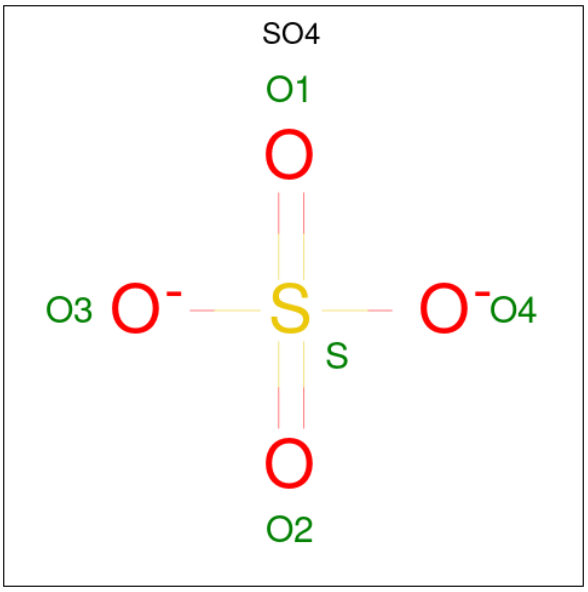
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P21695
A	-3	PRO	-	CLONING ARTIFACT	UNP P21695
A	-2	LEU	-	CLONING ARTIFACT	UNP P21695
A	-1	GLY	-	CLONING ARTIFACT	UNP P21695
A	0	SER	-	CLONING ARTIFACT	UNP P21695
A	1	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	38	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	144	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	148	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	181	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	233	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	235	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	323	MSE	MET	MODIFIED RESIDUE	UNP P21695
A	349	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	-4	GLY	-	CLONING ARTIFACT	UNP P21695
B	-3	PRO	-	CLONING ARTIFACT	UNP P21695
B	-2	LEU	-	CLONING ARTIFACT	UNP P21695
B	-1	GLY	-	CLONING ARTIFACT	UNP P21695
B	0	SER	-	CLONING ARTIFACT	UNP P21695
B	1	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	38	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	144	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	148	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	181	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	233	MSE	MET	MODIFIED RESIDUE	UNP P21695

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	235	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	323	MSE	MET	MODIFIED RESIDUE	UNP P21695
B	349	MSE	MET	MODIFIED RESIDUE	UNP P21695

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	A	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	B	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

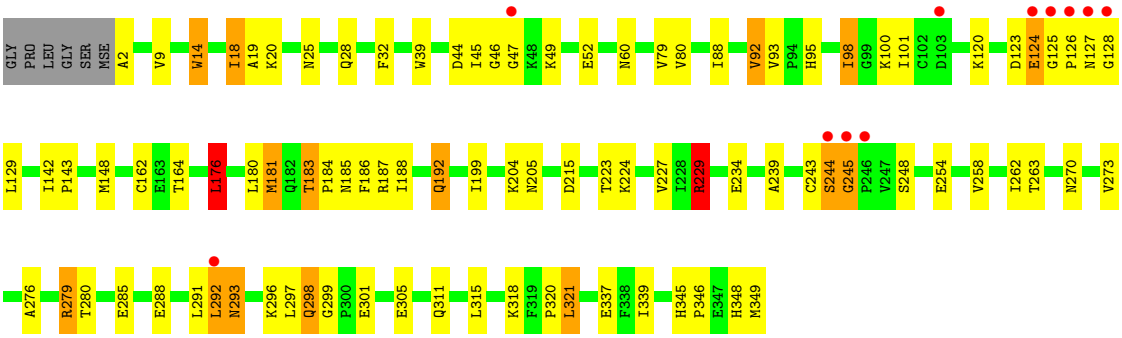
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	323	323	323	0	0
			Total	O		
3	B	328	328	328	0	0

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.

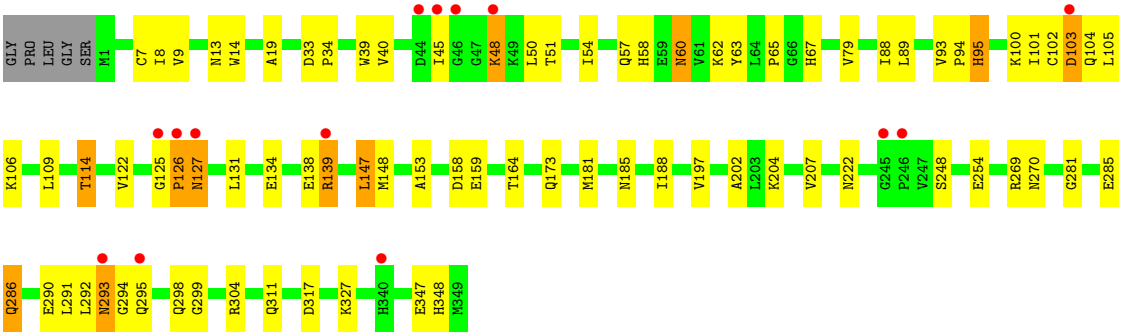
• Molecule 1: Glycerol-3-phosphate dehydrogenase [NAD+], cytoplasmic

Chain A:



• Molecule 1: Glycerol-3-phosphate dehydrogenase [NAD+], cytoplasmic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	113.49Å 113.49Å 155.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 32.06 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 99.6 (32.06-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 1.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.249 0.216 , 0.256	Depositor DCC
R_{free} test set	16176 reflections (9.79%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5977	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: SO4

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	0.70	3/2662 (0.1%)	0.85	5/3584 (0.1%)
1	B	0.79	4/2670 (0.1%)	0.92	10/3594 (0.3%)
All	All	0.74	7/5332 (0.1%)	0.88	15/7178 (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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	ARG	C-N	10.57	1.58	1.34
1	B	103	ASP	C-N	10.05	1.57	1.34
1	A	181	MSE	CG-SE	-5.94	1.75	1.95
1	A	349	MSE	SE-CE	-5.68	1.61	1.95
1	B	102	CYS	C-N	-5.64	1.21	1.34
1	B	181	MSE	CG-SE	-5.64	1.76	1.95
1	A	349	MSE	CG-SE	-5.01	1.78	1.95

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	GLU	O-C-N	-10.59	105.75	122.70
1	B	139	ARG	O-C-N	8.96	137.03	122.70
1	B	138	GLU	C-N-CA	8.63	143.27	121.70
1	B	103	ASP	CB-CA-C	7.79	125.99	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	GLY	N-CA-C	-7.73	93.77	113.10
1	B	138	GLU	CA-C-N	7.55	133.82	117.20
1	B	139	ARG	CA-C-N	-7.16	101.45	117.20
1	B	147	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	321	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	176	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	181	MSE	CG-SE-CE	-5.47	86.87	98.90
1	B	102	CYS	C-N-CA	-5.30	108.45	121.70
1	A	229	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	181	MSE	CG-SE-CE	-5.08	87.71	98.90
1	B	139	ARG	C-N-CA	-5.05	109.06	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	ASP	Mainchain

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	2624	0	2666	80	0
1	B	2632	0	2678	63	0
2	A	40	0	0	1	0
2	B	30	0	0	1	0
3	A	323	0	0	18	0
3	B	328	0	0	16	0
All	All	5977	0	5344	138	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 13.

All (138) 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:183:THR:HG22	1:A:185:ASN:H	1.18	1.04
1:A:279:ARG:HH11	1:A:279:ARG:HB3	1.15	1.03
1:B:100:LYS:O	1:B:104:GLN:HG3	1.56	1.02
1:A:183:THR:HG21	3:A:1256:HOH:O	1.70	0.90
1:A:291:LEU:O	1:A:292:LEU:HD13	1.75	0.85
1:B:159:GLU:HG3	3:B:1275:HOH:O	1.81	0.79
1:B:126:PRO:O	1:B:127:ASN:HB2	1.83	0.76
1:B:311:GLN:HB2	3:B:1328:HOH:O	1.86	0.75
1:B:207:VAL:HB	3:B:1197:HOH:O	1.87	0.75
1:A:44:ASP:HB3	3:A:1108:HOH:O	1.87	0.74
1:A:254:GLU:OE2	1:B:348:HIS:HE1	1.71	0.73
1:A:279:ARG:HH11	1:A:279:ARG:CB	1.98	0.73
1:B:39:TRP:CZ3	1:B:101:ILE:HD11	2.24	0.71
1:A:270:ASN:HD21	1:A:299:GLY:H	1.39	0.70
1:B:270:ASN:HD21	1:B:299:GLY:H	1.40	0.70
1:A:183:THR:HG22	1:A:185:ASN:N	2.00	0.69
1:A:95:HIS:O	1:A:98:ILE:HG23	1.92	0.69
1:A:120:LYS:HB2	3:A:1300:HOH:O	1.91	0.69
1:B:60:ASN:ND2	3:B:1122:HOH:O	2.26	0.69
1:A:348:HIS:HE1	1:B:254:GLU:OE2	1.77	0.68
1:B:114:THR:HG21	1:B:173:GLN:HE22	1.59	0.68
1:B:7:CYS:HB3	1:B:89:LEU:HD23	1.75	0.67
1:A:305:GLU:HG2	3:A:1119:HOH:O	1.95	0.67
1:B:114:THR:CG2	1:B:173:GLN:HE22	2.08	0.67
1:A:239:ALA:O	1:A:243:CYS:HB2	1.98	0.64
1:A:183:THR:CG2	1:A:185:ASN:H	2.04	0.63
1:A:296:LYS:HE3	3:A:1191:HOH:O	1.98	0.63
1:B:95:HIS:HD2	1:B:298:GLN:NE2	1.97	0.62
1:A:205:ASN:ND2	1:A:298:GLN:HG3	2.15	0.62
1:A:120:LYS:HA	3:A:1074:HOH:O	1.99	0.62
1:A:279:ARG:HB3	1:A:279:ARG:NH1	2.01	0.61
1:A:337:GLU:HG2	3:A:1178:HOH:O	2.00	0.61
1:A:39:TRP:CZ3	1:A:101:ILE:HD11	2.36	0.61
1:A:49:LYS:HB2	1:A:52:GLU:HG3	1.83	0.59
1:A:124:GLU:C	1:A:126:PRO:HD2	2.23	0.59
1:B:158:ASP:O	1:B:159:GLU:HB2	2.03	0.58
1:B:164:THR:HG22	1:B:188:ILE:HG12	1.86	0.57
1:A:181:MSE:HB2	1:A:188:ILE:HD11	1.85	0.57
1:A:339:ILE:HG12	3:A:1224:HOH:O	2.05	0.57
1:A:315:LEU:HD22	1:A:318:LYS:HG3	1.86	0.57
1:A:270:ASN:ND2	1:A:299:GLY:H	2.00	0.56
1:A:229:ARG:NH2	3:A:1060:HOH:O	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:VAL:HG21	1:A:292:LEU:HD21	1.87	0.56
1:B:63:TYR:N	3:B:1122:HOH:O	2.32	0.55
1:A:296:LYS:HG2	1:A:301:GLU:OE2	2.06	0.55
1:A:285:GLU:HA	1:A:288:GLU:OE1	2.07	0.55
1:B:106:LYS:HG3	1:B:139:ARG:O	2.06	0.54
1:B:79:VAL:HG22	1:B:105:LEU:HD21	1.90	0.53
1:B:126:PRO:O	1:B:127:ASN:CB	2.55	0.53
1:A:181:MSE:HB2	1:A:188:ILE:CD1	2.39	0.53
1:A:164:THR:HG22	1:A:188:ILE:HG12	1.90	0.53
1:A:276:ALA:HA	1:A:279:ARG:NH1	2.22	0.53
1:A:291:LEU:C	1:A:292:LEU:HD13	2.28	0.52
1:A:276:ALA:HA	1:A:279:ARG:HH12	1.74	0.52
1:B:67:HIS:HA	2:B:1010:SO4:O2	2.10	0.52
1:A:162:CYS:HB3	1:B:222:ASN:HB3	1.92	0.52
1:B:40:VAL:HB	1:B:51:THR:HG22	1.91	0.52
1:A:254:GLU:OE2	1:B:348:HIS:CE1	2.59	0.51
1:B:8:ILE:CD1	1:B:19:ALA:HA	2.40	0.51
1:B:317:ASP:HB2	3:B:1236:HOH:O	2.11	0.51
1:B:94:PRO:HG2	1:B:295:GLN:HE22	1.74	0.50
1:A:2:ALA:N	3:A:1059:HOH:O	2.44	0.50
1:A:20:LYS:NZ	2:A:1001:SO4:O3	2.40	0.50
1:B:286:GLN:OE1	1:B:290:GLU:OE2	2.29	0.50
1:A:129:LEU:HD21	1:A:199:ILE:HD13	1.94	0.50
1:B:65:PRO:HD2	3:B:1218:HOH:O	2.11	0.49
1:B:9:VAL:O	1:B:93:VAL:HG13	2.12	0.49
1:A:205:ASN:HD22	1:A:298:GLN:HG3	1.77	0.49
1:B:95:HIS:HD2	1:B:298:GLN:HE22	1.60	0.49
1:B:131:LEU:HB2	1:B:134:GLU:HG3	1.94	0.49
1:A:32:PHE:CZ	1:A:180:LEU:HB2	2.48	0.49
1:A:126:PRO:O	1:A:126:PRO:HG2	2.13	0.49
1:A:100:LYS:HG3	3:A:1297:HOH:O	2.12	0.49
1:B:122:VAL:HG13	1:B:202:ALA:HB1	1.93	0.48
1:A:183:THR:HG23	1:A:184:PRO:HD2	1.96	0.48
1:B:62:LYS:HB3	3:B:1122:HOH:O	2.12	0.48
1:A:293:ASN:ND2	3:A:1080:HOH:O	2.47	0.48
1:B:88:ILE:HA	1:B:114:THR:HG22	1.95	0.47
1:A:244:SER:O	1:A:245:GLY:O	2.32	0.47
1:B:89:LEU:HD11	1:B:109:LEU:HD22	1.96	0.47
1:A:18:ILE:HG22	1:A:19:ALA:N	2.28	0.47
1:A:125:GLY:O	1:A:127:ASN:N	2.47	0.47
1:B:295:GLN:HA	1:B:295:GLN:OE1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ASP:OD2	1:A:224:LYS:NZ	2.40	0.47
1:A:223:THR:O	1:A:227:VAL:HG23	2.15	0.47
1:B:62:LYS:HE2	1:B:63:TYR:OH	2.14	0.47
1:B:269:ARG:HH11	1:B:269:ARG:HB2	1.80	0.47
1:A:14:TRP:HE3	1:A:14:TRP:HA	1.80	0.47
1:A:123:ASP:HB3	1:A:126:PRO:HG3	1.97	0.47
1:A:348:HIS:CE1	1:B:254:GLU:OE2	2.63	0.47
1:A:80:VAL:HG23	3:A:1201:HOH:O	2.16	0.46
1:B:327:LYS:HD2	3:B:1113:HOH:O	2.15	0.46
1:B:7:CYS:HB3	1:B:89:LEU:CD2	2.45	0.46
1:A:88:ILE:HD11	1:A:176:LEU:CD1	2.46	0.46
1:A:148:MSE:HB3	3:A:1018:HOH:O	2.16	0.46
1:A:14:TRP:HA	1:A:14:TRP:CE3	2.52	0.45
1:A:298:GLN:NE2	1:A:298:GLN:H	2.14	0.45
1:A:44:ASP:C	1:A:45:ILE:HD12	2.37	0.45
1:A:345:HIS:CE1	1:A:346:PRO:HD2	2.52	0.45
1:B:292:LEU:O	1:B:293:ASN:OD1	2.35	0.45
1:A:45:ILE:O	1:A:45:ILE:HG22	2.17	0.44
1:B:57:GLN:NE2	3:B:1311:HOH:O	2.50	0.44
1:B:114:THR:OG1	1:B:173:GLN:NE2	2.50	0.44
1:B:285:GLU:HG3	3:B:1318:HOH:O	2.17	0.44
1:B:292:LEU:O	1:B:294:GLY:N	2.50	0.44
1:B:50:LEU:HD11	1:B:60:ASN:ND2	2.32	0.44
1:B:13:ASN:ND2	1:B:153:ALA:HB3	2.33	0.44
1:A:273:VAL:HG21	1:A:292:LEU:CD2	2.47	0.43
1:B:45:ILE:HG22	1:B:45:ILE:O	2.18	0.43
1:A:192:GLN:HE21	1:A:192:GLN:HB3	1.61	0.43
1:A:276:ALA:O	1:A:280:THR:HG23	2.18	0.43
1:B:125:GLY:O	1:B:126:PRO:C	2.57	0.43
1:B:33:ASP:HA	1:B:34:PRO:HD3	1.86	0.42
1:A:124:GLU:HA	3:A:1119:HOH:O	2.18	0.42
1:B:48:LYS:HA	3:B:1248:HOH:O	2.19	0.42
1:B:67:HIS:HE1	1:B:158:ASP:OD1	2.02	0.42
1:B:185:ASN:ND2	3:B:1084:HOH:O	2.51	0.42
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.92	0.42
1:B:281:GLY:HA2	3:B:1237:HOH:O	2.19	0.42
1:A:9:VAL:O	1:A:93:VAL:HG13	2.19	0.41
1:A:273:VAL:CG2	1:A:292:LEU:HD21	2.49	0.41
1:B:291:LEU:O	1:B:292:LEU:HD23	2.21	0.41
1:A:234:GLU:OE1	1:A:320:PRO:HD2	2.20	0.41
1:A:258:VAL:O	1:A:262:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HE2	1:B:63:TYR:CZ	2.55	0.41
1:B:114:THR:HB	3:B:1208:HOH:O	2.21	0.41
1:B:95:HIS:CD2	1:B:298:GLN:NE2	2.84	0.41
1:A:142:ILE:HA	1:A:143:PRO:HD3	1.76	0.41
1:A:47:GLY:HA2	3:A:1108:HOH:O	2.21	0.41
1:A:92:VAL:O	1:A:92:VAL:HG13	2.21	0.41
1:A:93:VAL:HG11	1:A:101:ILE:CD1	2.51	0.41
1:B:54:ILE:O	1:B:58:HIS:HA	2.21	0.41
1:B:347:GLU:HG2	3:B:1322:HOH:O	2.20	0.41
1:A:25:ASN:ND2	3:A:1231:HOH:O	2.53	0.41
1:B:148:MSE:HG3	1:B:197:VAL:HG12	2.03	0.40
1:A:183:THR:HB	1:A:186:PHE:HB3	2.04	0.40
1:A:123:ASP:OD2	1:A:126:PRO:HG3	2.22	0.40
1:A:46:GLY:HA3	3:A:1139:HOH: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	346/354 (98%)	331 (96%)	13 (4%)	2 (1%)	25	31
1	B	347/354 (98%)	332 (96%)	13 (4%)	2 (1%)	25	31
All	All	693/708 (98%)	663 (96%)	26 (4%)	4 (1%)	25	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	A	245	GLY
1	B	127	ASN
1	A	92	VAL

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	282/277 (102%)	260 (92%)	22 (8%)	12 16
1	B	283/277 (102%)	272 (96%)	11 (4%)	32 46
All	All	565/554 (102%)	532 (94%)	33 (6%)	20 27

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	TRP
1	A	18	ILE
1	A	28	GLN
1	A	60	ASN
1	A	79	VAL
1	A	98	ILE
1	A	124	GLU
1	A	176	LEU
1	A	183	THR
1	A	187	ARG
1	A	192	GLN
1	A	204	LYS
1	A	229	ARG
1	A	244	SER
1	A	248	SER
1	A	263	THR
1	A	279	ARG
1	A	292	LEU
1	A	293	ASN
1	A	298	GLN
1	A	311	GLN
1	A	321	LEU
1	B	14	TRP
1	B	48	LYS
1	B	60	ASN
1	B	95	HIS
1	B	114	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	126	PRO
1	B	147	LEU
1	B	204	LYS
1	B	248	SER
1	B	286	GLN
1	B	304	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	60	ASN
1	A	81	GLN
1	A	104	GLN
1	A	127	ASN
1	A	185	ASN
1	A	192	GLN
1	A	270	ASN
1	A	298	GLN
1	A	312	HIS
1	A	340	HIS
1	A	348	HIS
1	B	13	ASN
1	B	25	ASN
1	B	60	ASN
1	B	151	ASN
1	B	173	GLN
1	B	185	ASN
1	B	270	ASN
1	B	298	GLN
1	B	312	HIS
1	B	348	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	SO4	A	1013	-	4,4,4	0.86	0	6,6,6	0.15	0
2	SO4	B	1005	-	4,4,4	0.68	0	6,6,6	0.30	0
2	SO4	A	1003	-	4,4,4	0.71	0	6,6,6	0.32	0
2	SO4	A	1001	-	4,4,4	0.39	0	6,6,6	0.18	0
2	SO4	A	1004	-	4,4,4	0.79	0	6,6,6	0.18	0
2	SO4	A	1007	-	4,4,4	0.54	0	6,6,6	0.23	0
2	SO4	B	1010	-	4,4,4	0.58	0	6,6,6	0.32	0
2	SO4	A	1009	-	4,4,4	0.84	0	6,6,6	0.16	0
2	SO4	B	1011	-	4,4,4	0.71	0	6,6,6	0.19	0
2	SO4	B	1014	-	4,4,4	0.66	0	6,6,6	0.22	0
2	SO4	A	1002	-	4,4,4	0.72	0	6,6,6	0.23	0
2	SO4	A	1012	-	4,4,4	0.70	0	6,6,6	0.27	0
2	SO4	B	1006	-	4,4,4	0.73	0	6,6,6	0.59	0
2	SO4	B	1008	-	4,4,4	0.71	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1010	SO4	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	340/354 (96%)	-0.23	11 (3%)	47	54	18, 29, 55, 78	0
1	B	340/354 (96%)	-0.25	14 (4%)	37	44	18, 29, 51, 69	0
All	All	680/708 (96%)	-0.24	25 (3%)	41	48	18, 29, 53, 78	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	PRO	7.2
1	B	126	PRO	6.0
1	A	127	ASN	5.6
1	A	125	GLY	5.5
1	B	127	ASN	5.5
1	B	293	ASN	4.6
1	B	103	ASP	4.2
1	A	103	ASP	4.2
1	B	340	HIS	3.8
1	B	246	PRO	3.8
1	B	139	ARG	3.7
1	B	48	LYS	3.1
1	B	45	ILE	3.1
1	A	124	GLU	2.8
1	B	125	GLY	2.7
1	A	128	GLY	2.7
1	B	245	GLY	2.4
1	A	292	LEU	2.4
1	A	246	PRO	2.4
1	B	44	ASP	2.3
1	A	47	GLY	2.3
1	B	46	GLY	2.2
1	B	295	GLN	2.2
1	A	245	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	244	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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
2	SO4	B	1010	5/5	0.63	0.65	163,163,163,163	0
2	SO4	A	1002	5/5	0.67	0.58	146,146,146,147	0
2	SO4	A	1013	5/5	0.91	0.20	64,64,64,65	0
2	SO4	A	1004	5/5	0.91	0.17	81,82,82,83	0
2	SO4	B	1008	5/5	0.92	0.16	78,79,80,80	0
2	SO4	B	1014	5/5	0.92	0.30	96,96,97,97	0
2	SO4	B	1011	5/5	0.95	0.14	70,70,71,71	0
2	SO4	A	1001	5/5	0.96	0.42	127,127,128,129	0
2	SO4	A	1012	5/5	0.96	0.13	75,75,76,76	0
2	SO4	A	1003	5/5	0.96	0.12	56,58,59,59	0
2	SO4	B	1005	5/5	0.96	0.11	56,57,58,58	0
2	SO4	A	1007	5/5	0.97	0.24	86,86,87,87	0
2	SO4	B	1006	5/5	0.98	0.11	27,27,28,29	0
2	SO4	A	1009	5/5	0.99	0.09	26,26,28,29	0

6.5 Other polymers (i)

There are no such residues in this entry.