Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:07 AM EDT

PDB ID	:	3GG9
Title	:	CRYSTAL STRUCTURE OF putative D-3-phosphoglycerate dehydrogenase oxidoreductase from Ralstonia solanacearum
Authors	:	Patskovsky, Y.; Ramagopal, U.; Toro, R.; Morano, C.; Freeman, J.; Chang, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-02-27
Resolution	:	1.90 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:

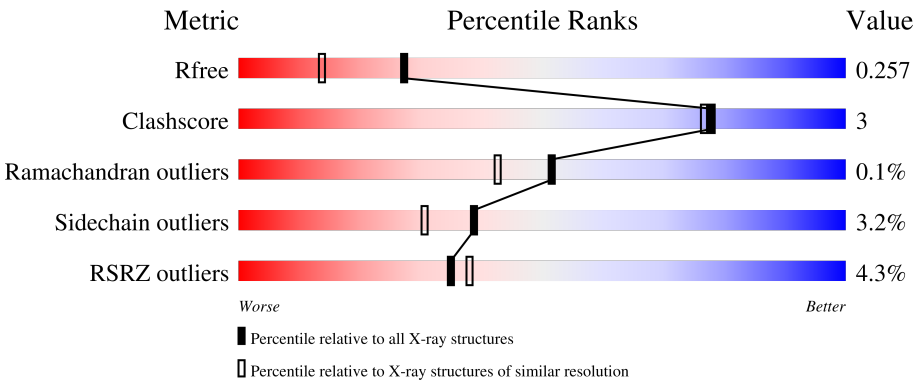
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	352	2%, 88%, 9%
1	B	352	3%, 90%, 7%
1	C	352	5%, 88%, 9%
1	D	352	6%, 88%, 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11868 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 d-3-phosphoglycerate dehydrogenase oxidoreductase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2737	1731	501	493	12	0	15	0
1	B	342	2698	1707	490	489	12	0	9	0
1	C	340	2696	1706	487	491	12	0	12	0
1	D	342	2695	1700	486	497	12	0	11	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	MET	SEE REMARK 999	UNP Q8Y3G4
A	61	LEU	ILE	SEE REMARK 999	UNP Q8Y3G4
A	240	SER	GLY	SEE REMARK 999	UNP Q8Y3G4
A	242	ILE	VAL	SEE REMARK 999	UNP Q8Y3G4
A	354	GLU	-	expression tag	UNP Q8Y3G4
A	355	GLY	-	expression tag	UNP Q8Y3G4
A	356	HIS	-	expression tag	UNP Q8Y3G4
A	357	HIS	-	expression tag	UNP Q8Y3G4
A	358	HIS	-	expression tag	UNP Q8Y3G4
A	359	HIS	-	expression tag	UNP Q8Y3G4
A	360	HIS	-	expression tag	UNP Q8Y3G4
A	361	HIS	-	expression tag	UNP Q8Y3G4
B	12	LEU	MET	SEE REMARK 999	UNP Q8Y3G4
B	61	LEU	ILE	SEE REMARK 999	UNP Q8Y3G4
B	240	SER	GLY	SEE REMARK 999	UNP Q8Y3G4
B	242	ILE	VAL	SEE REMARK 999	UNP Q8Y3G4
B	354	GLU	-	expression tag	UNP Q8Y3G4
B	355	GLY	-	expression tag	UNP Q8Y3G4
B	356	HIS	-	expression tag	UNP Q8Y3G4
B	357	HIS	-	expression tag	UNP Q8Y3G4
B	358	HIS	-	expression tag	UNP Q8Y3G4

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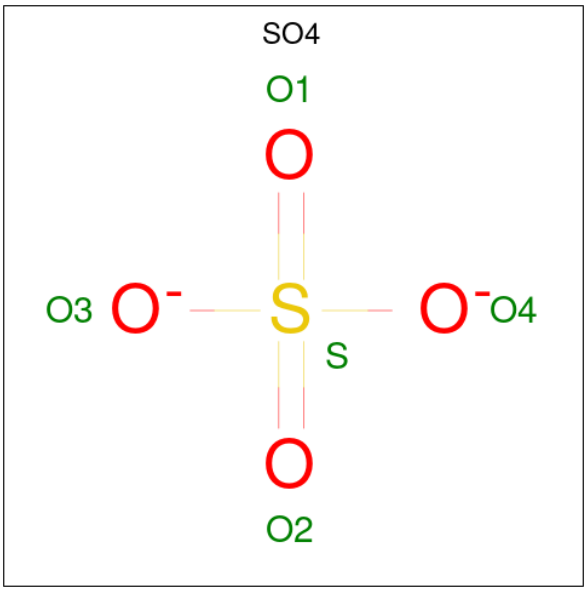
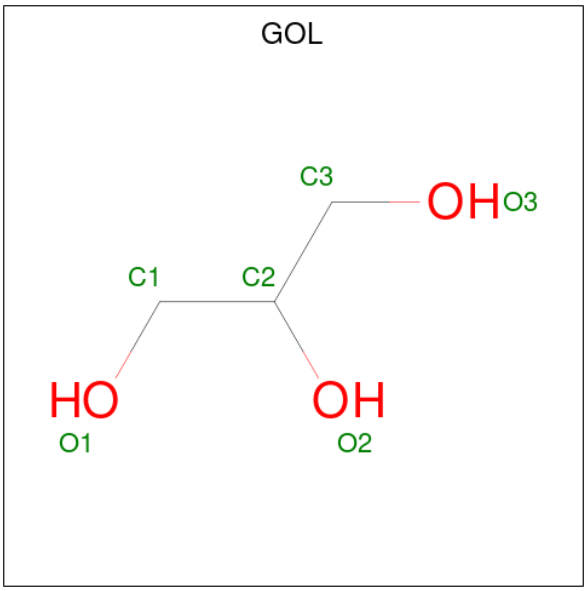
Chain	Residue	Modelled	Actual	Comment	Reference
B	359	HIS	-	expression tag	UNP Q8Y3G4
B	360	HIS	-	expression tag	UNP Q8Y3G4
B	361	HIS	-	expression tag	UNP Q8Y3G4
C	12	LEU	MET	SEE REMARK 999	UNP Q8Y3G4
C	61	LEU	ILE	SEE REMARK 999	UNP Q8Y3G4
C	240	SER	GLY	SEE REMARK 999	UNP Q8Y3G4
C	242	ILE	VAL	SEE REMARK 999	UNP Q8Y3G4
C	354	GLU	-	expression tag	UNP Q8Y3G4
C	355	GLY	-	expression tag	UNP Q8Y3G4
C	356	HIS	-	expression tag	UNP Q8Y3G4
C	357	HIS	-	expression tag	UNP Q8Y3G4
C	358	HIS	-	expression tag	UNP Q8Y3G4
C	359	HIS	-	expression tag	UNP Q8Y3G4
C	360	HIS	-	expression tag	UNP Q8Y3G4
C	361	HIS	-	expression tag	UNP Q8Y3G4
D	12	LEU	MET	SEE REMARK 999	UNP Q8Y3G4
D	61	LEU	ILE	SEE REMARK 999	UNP Q8Y3G4
D	240	SER	GLY	SEE REMARK 999	UNP Q8Y3G4
D	242	ILE	VAL	SEE REMARK 999	UNP Q8Y3G4
D	354	GLU	-	expression tag	UNP Q8Y3G4
D	355	GLY	-	expression tag	UNP Q8Y3G4
D	356	HIS	-	expression tag	UNP Q8Y3G4
D	357	HIS	-	expression tag	UNP Q8Y3G4
D	358	HIS	-	expression tag	UNP Q8Y3G4
D	359	HIS	-	expression tag	UNP Q8Y3G4
D	360	HIS	-	expression tag	UNP Q8Y3G4
D	361	HIS	-	expression tag	UNP Q8Y3G4

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



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

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



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	C	1	1	1	0	0
			Total	Cl		
4	D	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	291	291	291	0	0

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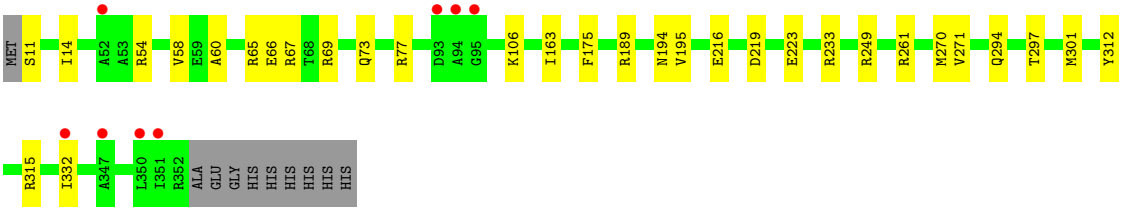
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	207	207	207	0	0
			Total	O		
5	C	198	198	198	0	0
			Total	O		
5	D	253	253	253	0	0

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.

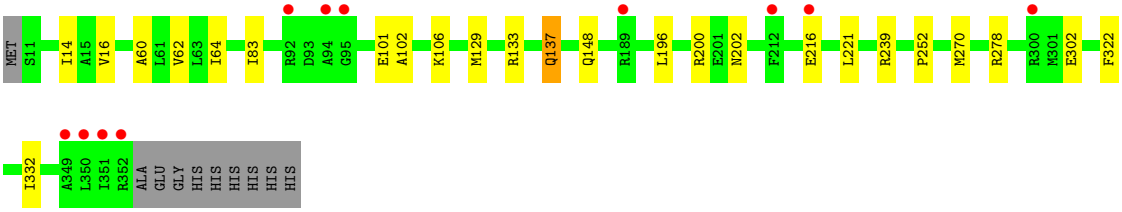
• Molecule 1: d-3-phosphoglycerate dehydrogenase oxidoreductase protein

Chain A:



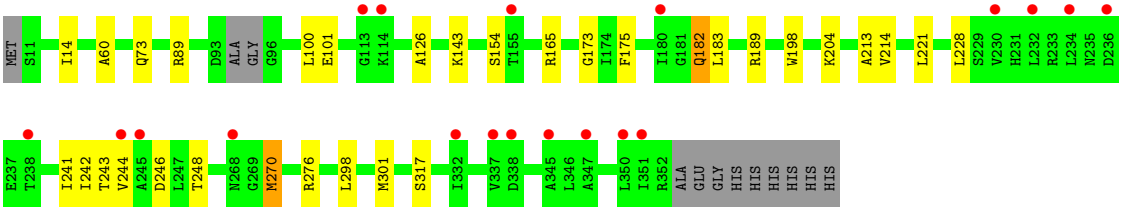
• Molecule 1: d-3-phosphoglycerate dehydrogenase oxidoreductase protein

Chain B:



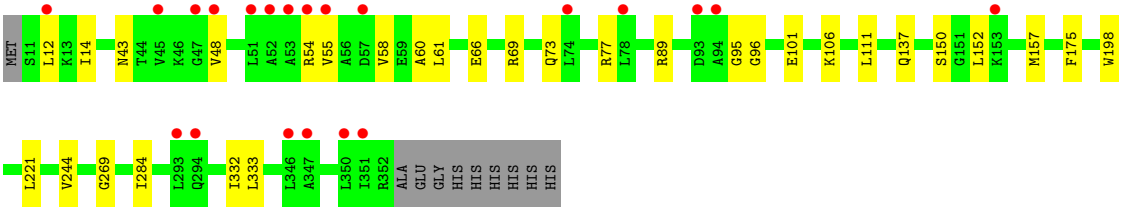
• Molecule 1: d-3-phosphoglycerate dehydrogenase oxidoreductase protein

Chain C:



• Molecule 1: d-3-phosphoglycerate dehydrogenase oxidoreductase protein

Chain D:


MET
S11
L12
K13
I14
N43
T44
V45
K46
G47
V48
L51
A52
A53
R54
V55
A56
D57
V58
E59
A60
L61
E66
R69
Q73
L74
R77
L78
R89
D93
A94
G95
G96
E101
K106
L111
Q137
S150
G151
L152
K153
M157
F175
W198
L221
V244
G269
I284
L293
Q294
I332
L333
L346
A347
L350
I351
R352
ALA
GLU
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.03Å 97.62Å 97.81Å 90.00° 114.96° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 45.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.90) 96.0 (45.95-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.199 , 0.261 0.199 , 0.257	Depositor DCC
R_{free} test set	3604 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11868	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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, GOL, CL

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	0.54	0/2825	0.67	1/3815 (0.0%)
1	B	0.48	0/2767	0.60	0/3738
1	C	0.46	0/2772	0.65	0/3745
1	D	0.51	0/2769	0.65	0/3747
All	All	0.50	0/11133	0.64	1/15045 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	NE-CZ-NH1	5.78	123.19	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	2737	0	2849	23	0
1	B	2698	0	2799	16	0
1	C	2696	0	2802	14	0
1	D	2695	0	2776	13	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	0	0	0
2	D	20	0	0	0	0
3	A	18	0	24	2	0
3	B	6	0	8	1	0
3	D	12	0	16	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	291	0	0	6	0
5	B	207	0	0	2	0
5	C	198	0	0	3	0
5	D	253	0	0	1	0
All	All	11868	0	11274	65	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 3.

All (65) 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:219[B]:ASP:OD1	1:A:249[B]:ARG:HD3	1.63	0.99
1:A:65[B]:ARG:HD3	1:A:312[B]:TYR:CE2	2.00	0.96
1:A:65[B]:ARG:HD3	1:A:312[B]:TYR:CD2	2.04	0.91
1:A:219[B]:ASP:OD1	1:A:249[B]:ARG:CD	2.22	0.87
1:C:213:ALA:HB1	5:C:847:HOH:O	1.83	0.78
1:B:137:GLN:HE21	1:B:137:GLN:H	1.31	0.78
1:B:83:ILE:HD11	1:B:332:ILE:HD11	1.72	0.71
1:C:270:MET:HG2	1:C:298:LEU:HD21	1.74	0.70
1:D:198:TRP:HB3	1:D:221:LEU:HD22	1.74	0.70
1:C:143[B]:LYS:NZ	5:C:669:HOH:O	2.24	0.70
1:B:129:MET:HE3	1:C:126:ALA:HA	1.74	0.70
1:A:65[B]:ARG:CD	1:A:312[B]:TYR:CD2	2.76	0.68
1:B:200:ARG:HB2	3:B:1:GOL:H2	1.75	0.67
1:D:244[A]:VAL:HG22	1:D:269:GLY:HA2	1.80	0.62
1:A:219[B]:ASP:OD1	1:A:249[B]:ARG:NE	2.32	0.61
1:A:77:ARG:HH11	1:A:77:ARG:HG3	1.65	0.61
1:A:297:THR:HG22	1:A:301:MET:CE	2.30	0.61
1:C:73[B]:GLN:HE21	1:C:73[B]:GLN:H	1.48	0.60
1:A:223:GLU:HG3	1:A:249[A]:ARG:HG2	1.83	0.59
1:D:14:ILE:HG12	1:D:60:ALA:HB3	1.85	0.58
1:C:248:THR:HG21	1:C:276:ARG:HH11	1.69	0.58
1:B:137:GLN:H	1:B:137:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244[A]:VAL:HG23	5:D:650:HOH:O	2.04	0.56
1:A:11:SER:N	5:A:543:HOH:O	2.39	0.55
1:A:216:GLU:OE2	1:C:165[B]:ARG:NH2	2.39	0.55
1:A:261[A]:ARG:NH1	5:A:937:HOH:O	2.28	0.55
1:A:297:THR:HG22	1:A:301:MET:HE2	1.89	0.53
1:B:83:ILE:CD1	1:B:332:ILE:HD11	2.37	0.52
1:A:14:ILE:HG12	1:A:60:ALA:HB3	1.92	0.51
1:B:200:ARG:HG2	1:B:200:ARG:HH21	1.74	0.51
1:A:189[A]:ARG:NH2	1:A:195:VAL:H	2.10	0.49
1:D:12:LEU:HD11	1:D:333:LEU:HD21	1.93	0.49
1:B:14:ILE:HG12	1:B:60:ALA:HB3	1.94	0.49
1:D:244[B]:VAL:HG13	1:D:269:GLY:HA2	1.94	0.47
1:D:111:LEU:HD21	1:D:332:ILE:HD13	1.97	0.47
1:D:137:GLN:HB3	1:D:150:SER:O	2.14	0.46
1:A:271:VAL:HG22	1:A:301:MET:HE1	1.98	0.46
1:A:315[B]:ARG:NH1	5:A:660:HOH:O	2.48	0.46
1:B:16:VAL:HG22	1:B:62:VAL:HB	1.98	0.46
1:A:66:GLU:OE2	1:A:261[B]:ARG:NH2	2.49	0.44
3:A:364:GOL:H11	5:A:530:HOH:O	2.16	0.44
1:C:243:THR:HG23	1:C:246:ASP:H	1.83	0.44
1:C:298:LEU:HA	1:C:301:MET:HE3	2.00	0.43
1:C:14:ILE:HG12	1:C:60:ALA:HB3	2.01	0.43
1:C:241:ILE:HG23	1:C:242:ILE:HG13	2.00	0.43
1:C:182:GLN:HG3	1:C:183:LEU:N	2.33	0.43
1:D:77:ARG:HH21	1:D:77:ARG:HG3	1.83	0.43
1:D:43:ASN:OD1	1:D:54:ARG:NH2	2.36	0.43
1:D:152:LEU:HB3	1:D:157:MET:HE1	1.99	0.43
1:B:133:ARG:HD3	5:B:932:HOH:O	2.19	0.42
1:C:198:TRP:HB3	1:C:221:LEU:HD22	2.01	0.42
1:C:173:GLY:O	1:C:228:LEU:HA	2.20	0.42
1:D:55:VAL:HG21	1:D:61:LEU:HD13	2.02	0.42
1:A:233:ARG:HA	3:A:364:GOL:H12	2.02	0.41
1:B:102:ALA:O	1:B:106:LYS:HG2	2.20	0.41
1:B:64[B]:ILE:HG13	1:B:322:PHE:HZ	1.86	0.41
1:B:252:PRO:HD3	1:B:278:ARG:CZ	2.51	0.41
1:A:106:LYS:CE	5:A:855:HOH:O	2.68	0.41
1:A:77:ARG:HG3	1:A:77:ARG:NH1	2.35	0.41
1:B:148:GLN:OE1	5:B:946:HOH:O	2.22	0.41
1:B:196:LEU:HB3	1:B:221:LEU:HD12	2.02	0.41
1:D:48:VAL:HG11	1:D:73:GLN:HG3	2.02	0.41
1:A:106:LYS:HD2	5:A:855:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:HB2	5:C:764: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	355/352 (101%)	348 (98%)	7 (2%)	0	100	100
1	B	349/352 (99%)	341 (98%)	8 (2%)	0	100	100
1	C	348/352 (99%)	338 (97%)	10 (3%)	0	100	100
1	D	351/352 (100%)	340 (97%)	9 (3%)	2 (1%)	25	15
All	All	1403/1408 (100%)	1367 (97%)	34 (2%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	GLY
1	D	95	GLY

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	295/288 (102%)	283 (96%)	12 (4%)	30	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	289/288 (100%)	282 (98%)	7 (2%)	49	43
1	C	292/288 (101%)	279 (96%)	13 (4%)	27	18
1	D	291/288 (101%)	282 (97%)	9 (3%)	40	32
All	All	1167/1152 (101%)	1126 (96%)	41 (4%)	39	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	ARG
1	A	54[B]	ARG
1	A	58	VAL
1	A	69	ARG
1	A	73[A]	GLN
1	A	73[B]	GLN
1	A	163[A]	ILE
1	A	163[B]	ILE
1	A	175	PHE
1	A	270	MET
1	A	294	GLN
1	A	332	ILE
1	B	101	GLU
1	B	137	GLN
1	B	202	ASN
1	B	216	GLU
1	B	239	ARG
1	B	270	MET
1	B	302	GLU
1	C	89	ARG
1	C	100	LEU
1	C	101	GLU
1	C	154	SER
1	C	175	PHE
1	C	182	GLN
1	C	189[A]	ARG
1	C	189[B]	ARG
1	C	204	LYS
1	C	214	VAL
1	C	244	VAL
1	C	270	MET
1	C	317	SER
1	D	58	VAL

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Mol	Chain	Res	Type
1	D	66	GLU
1	D	69	ARG
1	D	89[A]	ARG
1	D	89[B]	ARG
1	D	101	GLU
1	D	106	LYS
1	D	175	PHE
1	D	284	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	202	ASN
1	B	34	GLN
1	B	137	GLN
1	B	148	GLN
1	B	182	GLN
1	C	21	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 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
3	GOL	A	365	-	5,5,5	0.39	0	5,5,5	0.36	0
3	GOL	A	364	-	5,5,5	0.49	0	5,5,5	0.44	0
2	SO4	A	1	-	4,4,4	0.16	0	6,6,6	0.22	0
3	GOL	A	363	-	5,5,5	0.29	0	5,5,5	0.38	0
2	SO4	C	8	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	C	9	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	D	363	-	4,4,4	0.28	0	6,6,6	0.25	0
2	SO4	A	362	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	3	-	4,4,4	0.25	0	6,6,6	0.18	0
3	GOL	D	365	-	5,5,5	0.33	0	5,5,5	0.52	0
3	GOL	D	364	-	5,5,5	0.45	0	5,5,5	0.67	0
3	GOL	B	1	-	5,5,5	0.40	0	5,5,5	0.21	0
2	SO4	B	5	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	B	6	-	4,4,4	0.26	0	6,6,6	0.44	0
2	SO4	D	4	-	4,4,4	0.33	0	6,6,6	0.39	0
2	SO4	D	362	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	A	2	-	4,4,4	0.28	0	6,6,6	0.40	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
3	GOL	A	365	-	-	4/4/4/4	-
3	GOL	A	364	-	-	4/4/4/4	-
3	GOL	A	363	-	-	4/4/4/4	-
3	GOL	D	365	-	-	2/4/4/4	-
3	GOL	D	364	-	-	4/4/4/4	-
3	GOL	B	1	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	363	GOL	C1-C2-C3-O3
3	A	364	GOL	C1-C2-C3-O3
3	A	364	GOL	O2-C2-C3-O3
3	A	365	GOL	O2-C2-C3-O3
3	D	364	GOL	O1-C1-C2-C3
3	D	365	GOL	O1-C1-C2-O2
3	D	365	GOL	O1-C1-C2-C3
3	D	364	GOL	O1-C1-C2-O2
3	A	363	GOL	O1-C1-C2-C3
3	A	364	GOL	O1-C1-C2-C3
3	A	365	GOL	O1-C1-C2-C3
3	A	365	GOL	C1-C2-C3-O3
3	D	364	GOL	C1-C2-C3-O3
3	A	363	GOL	O1-C1-C2-O2
3	D	364	GOL	O2-C2-C3-O3
3	A	364	GOL	O1-C1-C2-O2
3	A	365	GOL	O1-C1-C2-O2
3	A	363	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	364	GOL	2	0
3	B	1	GOL	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	342/352 (97%)	-0.11	8 (2%)	60	63	17, 32, 57, 103	0
1	B	342/352 (97%)	-0.05	11 (3%)	47	50	21, 39, 67, 89	0
1	C	340/352 (96%)	0.43	19 (5%)	24	27	27, 47, 68, 94	0
1	D	342/352 (97%)	0.21	21 (6%)	21	24	18, 35, 66, 92	0
All	All	1366/1408 (97%)	0.12	59 (4%)	35	38	17, 38, 66, 103	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	351	ILE	6.5
1	A	351	ILE	6.0
1	B	94	ALA	4.9
1	B	350	LEU	4.6
1	B	351	ILE	4.4
1	A	95	GLY	4.3
1	D	51	LEU	4.3
1	A	94	ALA	4.2
1	D	52	ALA	4.0
1	C	350	LEU	3.9
1	D	350	LEU	3.8
1	B	95	GLY	3.6
1	D	346	LEU	3.5
1	C	245	ALA	3.5
1	C	332	ILE	3.4
1	D	351	ILE	3.3
1	C	180	ILE	3.3
1	D	48	VAL	3.3
1	C	232	LEU	3.2
1	D	54	ARG	3.1
1	D	47	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	3.1
1	C	155	THR	3.0
1	C	337	VAL	3.0
1	D	293	LEU	3.0
1	D	347	ALA	2.9
1	C	236	ASP	2.9
1	B	349	ALA	2.8
1	B	300	ARG	2.8
1	C	345	ALA	2.8
1	A	332	ILE	2.7
1	B	212	PHE	2.7
1	D	74	LEU	2.7
1	C	114	LYS	2.6
1	C	244	VAL	2.6
1	D	57[A]	ASP	2.6
1	C	113	GLY	2.6
1	A	93	ASP	2.6
1	D	294	GLN	2.6
1	C	268[A]	ASN	2.4
1	A	52	ALA	2.4
1	D	93[A]	ASP	2.4
1	D	78	LEU	2.4
1	D	53	ALA	2.3
1	D	45	VAL	2.3
1	D	153	LYS	2.3
1	D	94	ALA	2.3
1	C	230	VAL	2.3
1	B	352	ARG	2.3
1	A	347	ALA	2.3
1	C	347	ALA	2.3
1	B	216	GLU	2.2
1	D	12	LEU	2.2
1	B	92[A]	ARG	2.1
1	C	238	THR	2.1
1	C	234	LEU	2.1
1	D	55	VAL	2.1
1	B	189[A]	ARG	2.0
1	C	338	ASP	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	GOL	D	365	6/6	0.50	0.30	52,68,74,76	0
2	SO4	D	363	5/5	0.68	0.23	41,43,54,60	5
3	GOL	D	364	6/6	0.72	0.20	41,53,55,57	0
3	GOL	A	365	6/6	0.78	0.17	57,62,65,66	0
2	SO4	C	9	5/5	0.81	0.20	36,41,47,56	5
3	GOL	B	1	6/6	0.86	0.17	82,89,91,94	0
2	SO4	B	6	5/5	0.88	0.10	60,66,72,79	0
3	GOL	A	364	6/6	0.91	0.16	38,47,55,56	0
2	SO4	C	8	5/5	0.92	0.21	35,41,50,51	5
3	GOL	A	363	6/6	0.96	0.11	31,42,50,51	0
2	SO4	D	4	5/5	0.96	0.07	40,41,51,54	0
2	SO4	A	362	5/5	0.96	0.08	70,70,71,78	0
2	SO4	B	5	5/5	0.97	0.15	59,60,73,73	0
2	SO4	A	2	5/5	0.97	0.07	40,43,50,55	0
4	CL	C	1	1/1	0.97	0.06	47,47,47,47	0
2	SO4	D	362	5/5	0.98	0.08	25,29,44,45	5
4	CL	D	1	1/1	0.98	0.08	39,39,39,39	0
2	SO4	D	3	5/5	0.99	0.06	50,54,60,65	0
2	SO4	A	1	5/5	0.99	0.09	40,42,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.