Full wwPDB X-ray Structure Validation Report (i)

Apr 25, 2026 – 03:29 PM EDT

PDB ID	:	3R0K / pdb_00003r0k
Title	:	Crystal structure of NYSGRC enolase target 200555, a putative dipeptide epimerase from Francisella philomiragia : Tartrate bound, no Mg
Authors	:	Vetting, M.W.; Hillerich, B.; Seidel, R.D.; Zencheck, W.D.; Toro, R.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-03-08
Resolution	:	2.00 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:

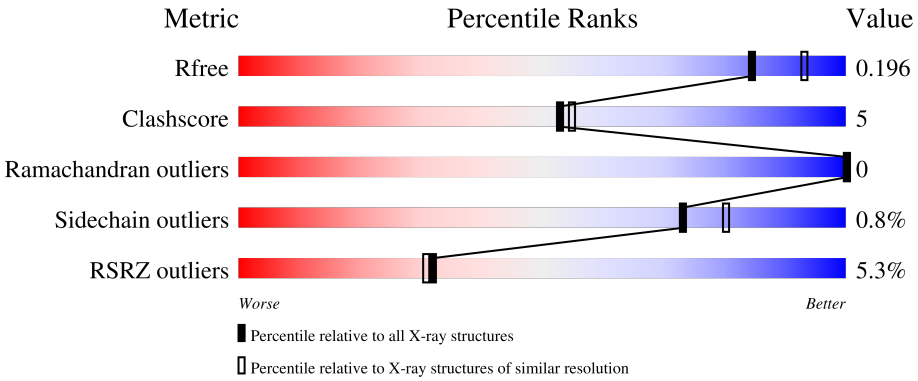
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	379	7% 81% 12% 6%
1	B	379	2% 89% 7% .

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	TAR	A	381	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6172 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 Enzyme of enolase superfamily.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2744	1759	442	531	4	8			
1	B	364	Total	C	N	O	S	Se	0	0	0
			2810	1796	456	546	4	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP B0TZW0
A	2	VAL	-	expression tag	UNP B0TZW0
A	358	ALA	-	expression tag	UNP B0TZW0
A	359	GLU	-	expression tag	UNP B0TZW0
A	360	ASN	-	expression tag	UNP B0TZW0
A	361	LEU	-	expression tag	UNP B0TZW0
A	362	TYR	-	expression tag	UNP B0TZW0
A	363	PHE	-	expression tag	UNP B0TZW0
A	364	GLN	-	expression tag	UNP B0TZW0
A	365	SER	-	expression tag	UNP B0TZW0
A	366	HIS	-	expression tag	UNP B0TZW0
A	367	HIS	-	expression tag	UNP B0TZW0
A	368	HIS	-	expression tag	UNP B0TZW0
A	369	HIS	-	expression tag	UNP B0TZW0
A	370	HIS	-	expression tag	UNP B0TZW0
A	371	HIS	-	expression tag	UNP B0TZW0
A	372	TRP	-	expression tag	UNP B0TZW0
A	373	SER	-	expression tag	UNP B0TZW0
A	374	HIS	-	expression tag	UNP B0TZW0
A	375	PRO	-	expression tag	UNP B0TZW0
A	376	GLN	-	expression tag	UNP B0TZW0
A	377	PHE	-	expression tag	UNP B0TZW0
A	378	GLU	-	expression tag	UNP B0TZW0
A	379	LYS	-	expression tag	UNP B0TZW0
B	1	MSE	-	expression tag	UNP B0TZW0

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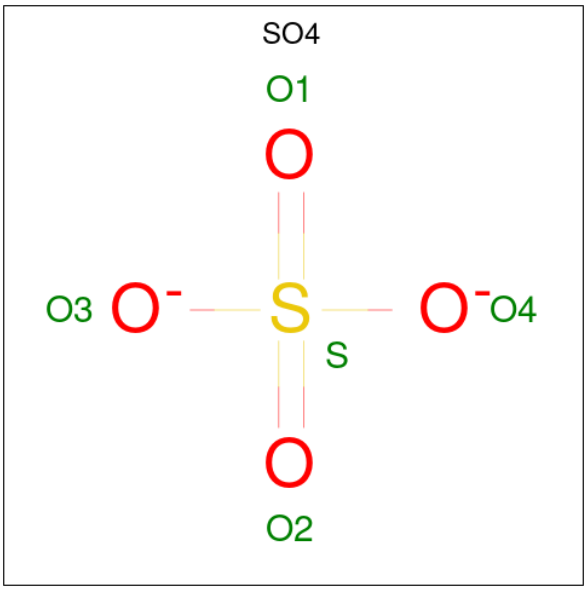
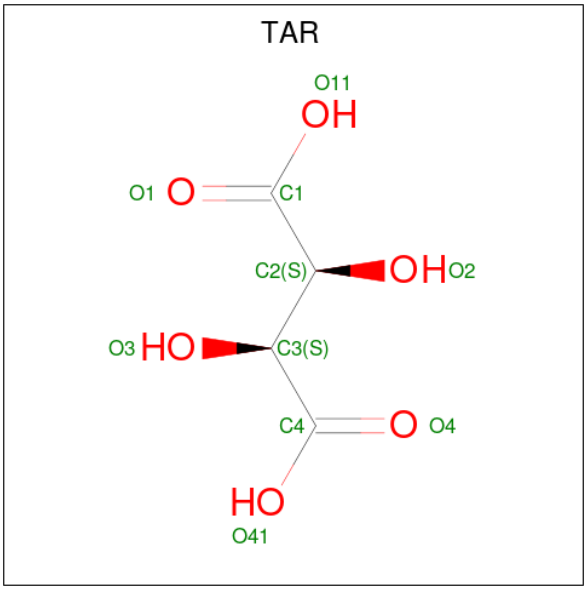
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	-	expression tag	UNP B0TZW0
B	358	ALA	-	expression tag	UNP B0TZW0
B	359	GLU	-	expression tag	UNP B0TZW0
B	360	ASN	-	expression tag	UNP B0TZW0
B	361	LEU	-	expression tag	UNP B0TZW0
B	362	TYR	-	expression tag	UNP B0TZW0
B	363	PHE	-	expression tag	UNP B0TZW0
B	364	GLN	-	expression tag	UNP B0TZW0
B	365	SER	-	expression tag	UNP B0TZW0
B	366	HIS	-	expression tag	UNP B0TZW0
B	367	HIS	-	expression tag	UNP B0TZW0
B	368	HIS	-	expression tag	UNP B0TZW0
B	369	HIS	-	expression tag	UNP B0TZW0
B	370	HIS	-	expression tag	UNP B0TZW0
B	371	HIS	-	expression tag	UNP B0TZW0
B	372	TRP	-	expression tag	UNP B0TZW0
B	373	SER	-	expression tag	UNP B0TZW0
B	374	HIS	-	expression tag	UNP B0TZW0
B	375	PRO	-	expression tag	UNP B0TZW0
B	376	GLN	-	expression tag	UNP B0TZW0
B	377	PHE	-	expression tag	UNP B0TZW0
B	378	GLU	-	expression tag	UNP B0TZW0
B	379	LYS	-	expression tag	UNP B0TZW0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



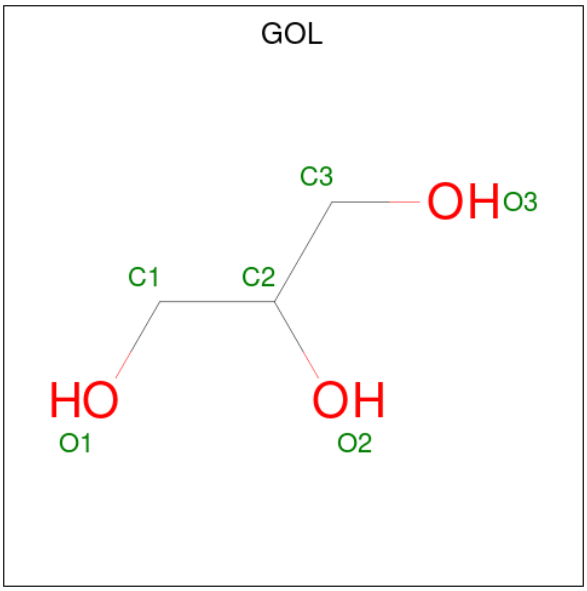
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

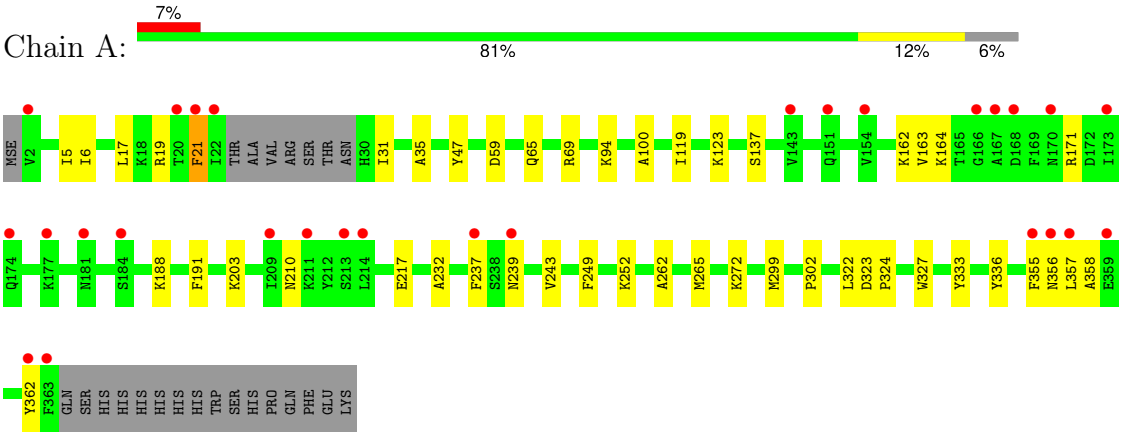
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	353	Total O 353 353	0	0

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.

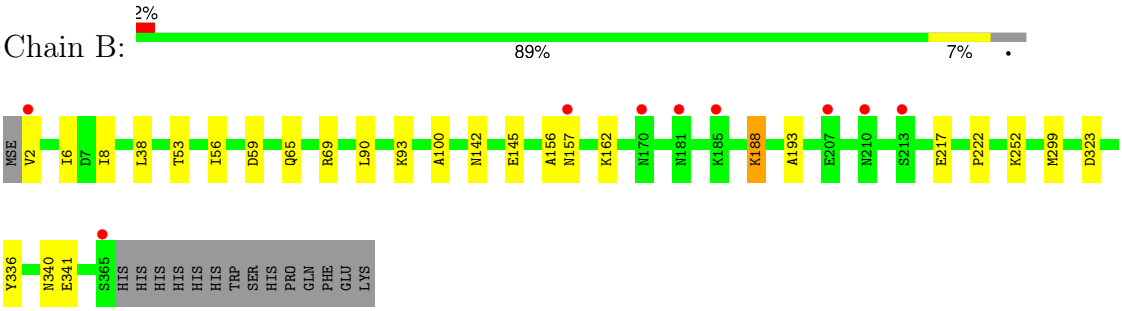
• Molecule 1: Enzyme of enolase superfamily

Chain A:



• Molecule 1: Enzyme of enolase superfamily

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.00Å 121.00Å 148.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.10 – 2.00 28.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.10-2.00) 99.9 (28.10-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	9.38 (at 1.99Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.165 , 0.197 0.164 , 0.196	Depositor DCC
R_{free} test set	3776 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 60.4	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	0.95	EDS
Total number of atoms	6172	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAR, GOL, 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	0.45	0/2775	0.80	3/3738 (0.1%)
1	B	0.50	0/2842	0.83	4/3831 (0.1%)
All	All	0.48	0/5617	0.82	7/7569 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	MSE	N-CA-C	-5.99	97.93	108.23
1	B	336	TYR	N-CA-C	5.92	121.41	113.72
1	B	323	ASP	N-CA-C	5.71	122.42	109.81
1	A	299	MSE	N-CA-C	-5.61	98.58	108.23
1	A	323	ASP	N-CA-C	5.51	122.00	109.81
1	A	6	ILE	N-CA-C	5.20	117.90	112.90
1	B	6	ILE	N-CA-C	5.15	117.85	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2744	0	2795	36	0
1	B	2810	0	2861	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	1	0
2	B	20	0	0	0	0
3	A	10	0	4	0	0
4	A	6	0	8	0	0
4	B	18	0	24	4	0
5	A	206	0	0	0	0
5	B	353	0	0	1	0
All	All	6172	0	5692	56	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 (56) 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:65:GLN:HE21	1:A:69:ARG:NH1	1.71	0.88
1:B:65:GLN:HE22	1:B:69:ARG:NE	1.74	0.86
1:B:65:GLN:NE2	1:B:69:ARG:NE	2.25	0.84
1:A:119:ILE:HB	1:A:123:LYS:HD2	1.69	0.73
1:A:163:VAL:CG2	1:A:191:PHE:CD1	2.78	0.67
1:B:65:GLN:NE2	1:B:69:ARG:CZ	2.58	0.66
1:A:163:VAL:HG21	1:A:191:PHE:CE1	2.29	0.66
1:B:65:GLN:HE22	1:B:69:ARG:CD	2.11	0.63
1:A:65:GLN:HE21	1:A:69:ARG:CZ	2.12	0.63
1:A:210:ASN:HD21	1:A:239:ASN:ND2	1.98	0.62
1:A:35:ALA:HB1	1:A:357:LEU:HD21	1.83	0.60
1:A:163:VAL:HG23	1:A:191:PHE:CD1	2.38	0.59
1:A:47:TYR:CD2	1:A:357:LEU:HD22	2.37	0.59
1:A:21:PHE:HB2	1:A:327:TRP:CH2	2.41	0.56
1:A:188:LYS:HD2	1:A:217:GLU:OE1	2.06	0.55
1:A:210:ASN:HD21	1:A:239:ASN:HD21	1.53	0.55
1:B:65:GLN:HE22	1:B:69:ARG:CZ	2.21	0.54
1:A:322:LEU:C	1:A:324:PRO:HD2	2.33	0.54
1:A:243:VAL:HG22	1:A:265:MSE:HB3	1.89	0.53
1:A:137:SER:HB3	1:A:162:LYS:HE2	1.91	0.51
1:A:59:ASP:CG	1:A:100:ALA:HB3	2.35	0.51
1:B:193:ALA:HB3	1:B:222:PRO:HA	1.92	0.51
1:A:19:ARG:HG3	1:A:327:TRP:CZ3	2.47	0.50
1:A:162:LYS:HE3	1:A:164:LYS:HE2	1.93	0.50
1:B:156:ALA:O	1:B:157:ASN:HB2	2.11	0.50
1:B:90:LEU:O	1:B:93:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:TYR:CE2	1:A:355:PHE:HB3	2.48	0.49
1:B:2:VAL:HG23	1:B:2:VAL:O	2.13	0.48
1:A:17:LEU:HD21	1:A:31:ILE:HG13	1.96	0.48
1:B:142:ASN:OD1	1:B:145:GLU:HG3	2.13	0.48
1:A:163:VAL:HG21	1:A:191:PHE:CD1	2.48	0.47
1:A:65:GLN:HE21	1:A:69:ARG:HH12	1.59	0.47
1:A:21:PHE:CB	1:A:327:TRP:CZ3	2.99	0.46
1:B:59:ASP:CG	1:B:100:ALA:HB3	2.40	0.46
1:A:94:LYS:HD3	4:B:385:GOL:H12	1.97	0.46
1:A:137:SER:CB	1:A:162:LYS:HE2	2.45	0.46
1:B:188:LYS:HE2	1:B:217:GLU:OE1	2.15	0.46
1:B:156:ALA:CB	4:B:386:GOL:H31	2.46	0.46
1:B:53:THR:HG21	1:B:56:ILE:HD12	1.99	0.45
1:A:203:LYS:HG2	1:A:237:PHE:CE2	2.50	0.45
1:B:90:LEU:HA	1:B:93:LYS:HD2	1.98	0.45
1:A:358:ALA:HA	1:A:362:TYR:HD2	1.82	0.44
1:B:340:ASN:O	1:B:341:GLU:C	2.60	0.44
1:A:69:ARG:HD3	2:A:380:SO4:O1	2.17	0.44
1:B:162:LYS:HE2	5:B:731:HOH:O	2.17	0.44
1:B:8:ILE:HG12	1:B:38:LEU:CD2	2.48	0.44
1:A:302:PRO:HB3	1:A:333:TYR:HB3	2.01	0.43
1:A:47:TYR:HD2	1:A:357:LEU:HD22	1.81	0.43
1:A:94:LYS:NZ	4:B:385:GOL:H32	2.34	0.42
1:A:232:ALA:HA	1:A:262:ALA:HA	2.01	0.42
1:B:156:ALA:HB2	4:B:386:GOL:H31	2.01	0.42
1:A:5:ILE:HD12	1:A:5:ILE:N	2.35	0.42
1:A:171:ARG:HD3	1:A:171:ARG:C	2.45	0.42
1:A:163:VAL:HG23	1:A:191:PHE:HD1	1.83	0.41
1:A:249:PHE:HA	1:A:272:LYS:HB3	2.03	0.40
1:B:8:ILE:HG12	1:B:38:LEU:HD22	2.03	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	351/379 (93%)	345 (98%)	6 (2%)	0	100	100
1	B	362/379 (96%)	356 (98%)	6 (2%)	0	100	100
All	All	713/758 (94%)	701 (98%)	12 (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	298/312 (96%)	295 (99%)	3 (1%)	68	75
1	B	306/312 (98%)	304 (99%)	2 (1%)	76	82
All	All	604/624 (97%)	599 (99%)	5 (1%)	73	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	PHE
1	A	252	LYS
1	A	356	ASN
1	B	188	LYS
1	B	252	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	204	GLN
1	A	210	ASN
1	B	65	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	B	382	-	4,4,4	0.22	0	6,6,6	0.05	0
4	GOL	B	385	-	5,5,5	0.36	0	5,5,5	0.30	0
2	SO4	B	381	-	4,4,4	0.31	0	6,6,6	0.31	0
2	SO4	A	380	-	4,4,4	0.23	0	6,6,6	0.15	0
4	GOL	B	386	-	5,5,5	0.43	0	5,5,5	0.64	0
4	GOL	B	384	-	5,5,5	0.49	0	5,5,5	0.21	0
3	TAR	A	381	-	9,9,9	1.58	2 (22%)	12,12,12	1.77	4 (33%)
2	SO4	B	383	-	4,4,4	0.24	0	6,6,6	0.15	0
4	GOL	A	382	-	5,5,5	0.39	0	5,5,5	0.13	0
2	SO4	B	380	-	4,4,4	0.22	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	385	-	-	2/4/4/4	-
4	GOL	B	386	-	-	2/4/4/4	-
4	GOL	B	384	-	-	0/4/4/4	-
3	TAR	A	381	-	-	11/12/12/12	-
4	GOL	A	382	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	381	TAR	O2-C2	-2.15	1.38	1.42
3	A	381	TAR	O3-C3	-2.06	1.38	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	381	TAR	O41-C4-C3	2.99	121.62	113.31
3	A	381	TAR	O41-C4-O4	-2.86	117.58	124.08
3	A	381	TAR	O11-C1-C2	2.65	120.67	113.31
3	A	381	TAR	O11-C1-O1	-2.08	119.36	124.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	386	GOL	O1-C1-C2-C3
3	A	381	TAR	O3-C3-C4-O4
3	A	381	TAR	O3-C3-C4-O41
4	B	385	GOL	O1-C1-C2-C3
3	A	381	TAR	C2-C3-C4-O41
4	B	386	GOL	O1-C1-C2-O2
3	A	381	TAR	C2-C3-C4-O4
3	A	381	TAR	C1-C2-C3-O3
4	B	385	GOL	O1-C1-C2-O2
3	A	381	TAR	C1-C2-C3-C4
3	A	381	TAR	O1-C1-C2-C3
3	A	381	TAR	O2-C2-C3-O3
3	A	381	TAR	O11-C1-C2-C3
3	A	381	TAR	O11-C1-C2-O2
3	A	381	TAR	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	385	GOL	2	0
2	A	380	SO4	1	0
4	B	386	GOL	2	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, 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	347/379 (91%)	0.19	28 (8%)	18	17	10, 27, 61, 90	0
1	B	356/379 (93%)	-0.38	9 (2%)	58	58	9, 21, 41, 67	0
All	All	703/758 (92%)	-0.10	37 (5%)	32	31	9, 23, 54, 90	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	5.6
1	A	170	ASN	5.0
1	A	181	ASN	4.7
1	B	213	SER	4.0
1	A	357	LEU	3.8
1	B	170	ASN	3.6
1	B	2	VAL	3.6
1	A	213	SER	3.6
1	B	210	ASN	3.4
1	A	174	GLN	3.2
1	A	21	PHE	3.1
1	A	211	LYS	3.1
1	A	363	PHE	3.0
1	B	181	ASN	2.7
1	A	168	ASP	2.7
1	A	20	THR	2.7
1	A	239	ASN	2.6
1	A	166	GLY	2.5
1	A	173	ILE	2.5
1	A	209	ILE	2.5
1	A	167	ALA	2.4
1	B	365	SER	2.4
1	A	143	VAL	2.4
1	B	185	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.3
1	A	2	VAL	2.3
1	A	154	VAL	2.3
1	A	355	PHE	2.3
1	B	157	ASN	2.3
1	A	359	GLU	2.2
1	A	356	ASN	2.2
1	A	177	LYS	2.2
1	A	237	PHE	2.2
1	A	184	SER	2.2
1	A	362	TYR	2.1
1	A	151	GLN	2.1
1	B	207	GLU	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 oligosaccharides 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, 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	B-factors(Å^2)	Q<0.9
4	GOL	B	385	6/6	0.76	0.24	52,56,61,70	0
3	TAR	A	381	10/10	0.79	0.16	39,55,64,65	0
2	SO4	A	380	5/5	0.85	0.12	65,67,71,73	0
4	GOL	B	386	6/6	0.87	0.19	35,39,43,44	0
2	SO4	B	381	5/5	0.91	0.12	34,36,41,46	0
2	SO4	B	383	5/5	0.92	0.16	54,55,57,61	0
4	GOL	A	382	6/6	0.92	0.09	24,26,27,30	0
2	SO4	B	382	5/5	0.93	0.14	36,40,44,48	0
4	GOL	B	384	6/6	0.93	0.10	19,23,24,26	0
2	SO4	B	380	5/5	0.98	0.09	28,29,34,36	0

6.5 Other polymers (i)

There are no such residues in this entry.