



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 10:03 PM EST

PDB ID : 4ZQR
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Mycobacterium tuberculosis
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Kavitha, M.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2015-05-11
Resolution : 1.69 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

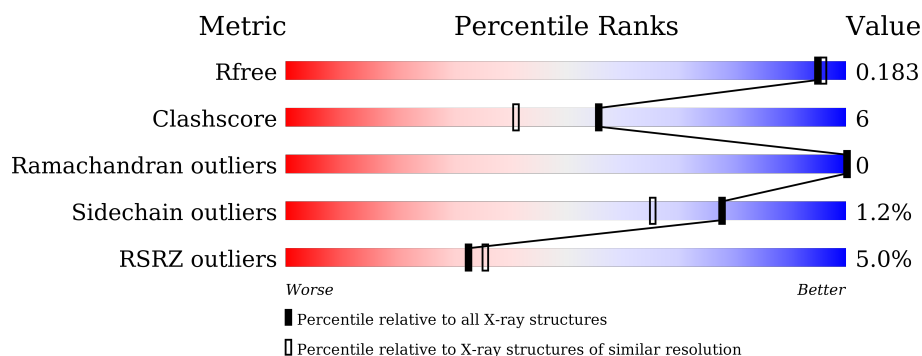
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	407	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>12%</div> </div> </div>
1	B	407	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>12%</div> </div> </div>
1	C	407	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>12%</div> </div> </div>
1	D	407	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGO	A	602	-	-	-	X
3	PGO	A	605	-	-	-	X
3	PGO	B	606	-	-	-	X
3	PGO	B	607	-	-	X	X
3	PGO	C	601	-	-	X	X
3	PGO	C	603	-	-	-	X
3	PGO	C	607	-	-	X	X
3	PGO	D	601[A]	-	-	X	X
3	PGO	D	601[B]	-	-	X	X
3	PGO	D	604	-	-	-	X
3	PGO	D	605	-	-	X	-
3	PGO	D	606	-	-	X	X
4	GOL	A	607	-	-	-	X
4	GOL	A	608	-	-	-	X
4	GOL	A	610	-	-	-	X
4	GOL	B	604	-	-	X	X
4	GOL	B	608	-	-	-	X
4	GOL	C	604	-	-	-	X
4	GOL	C	606	-	-	-	X
4	GOL	D	602	-	-	-	X
4	GOL	D	607	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11793 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.

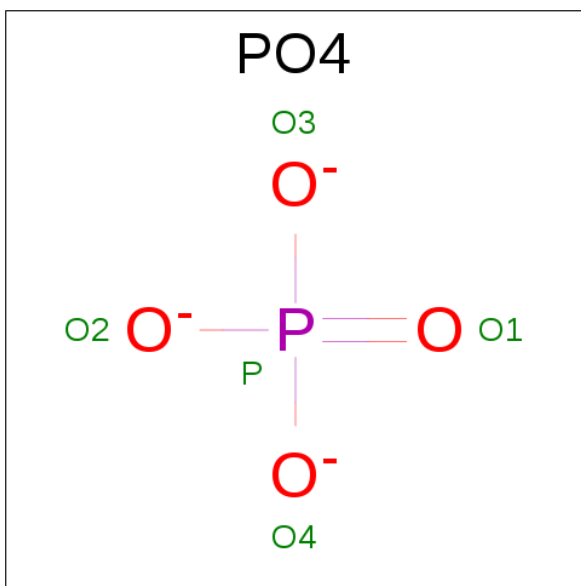
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	22	0
			2714	1697	487	511	19			
1	B	357	Total	C	N	O	S	0	20	0
			2694	1687	481	508	18			
1	C	358	Total	C	N	O	S	0	24	0
			2724	1703	488	515	18			
1	D	357	Total	C	N	O	S	0	21	0
			2698	1690	482	508	18			

There are 20 discrepancies between the modelled and reference sequences:

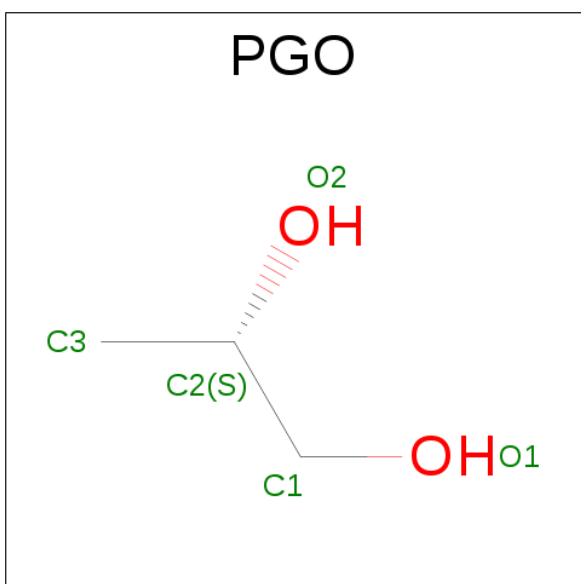
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P9WKI7
A	-1	ASN	-	expression tag	UNP P9WKI7
A	0	ALA	-	expression tag	UNP P9WKI7
A	126	GLY	-	linker	UNP P9WKI7
A	127	GLY	-	linker	UNP P9WKI7
B	-2	SER	-	expression tag	UNP P9WKI7
B	-1	ASN	-	expression tag	UNP P9WKI7
B	0	ALA	-	expression tag	UNP P9WKI7
B	126	GLY	-	linker	UNP P9WKI7
B	127	GLY	-	linker	UNP P9WKI7
C	-2	SER	-	expression tag	UNP P9WKI7
C	-1	ASN	-	expression tag	UNP P9WKI7
C	0	ALA	-	expression tag	UNP P9WKI7
C	126	GLY	-	linker	UNP P9WKI7
C	127	GLY	-	linker	UNP P9WKI7
D	-2	SER	-	expression tag	UNP P9WKI7
D	-1	ASN	-	expression tag	UNP P9WKI7
D	0	ALA	-	expression tag	UNP P9WKI7
D	126	GLY	-	linker	UNP P9WKI7
D	127	GLY	-	linker	UNP P9WKI7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



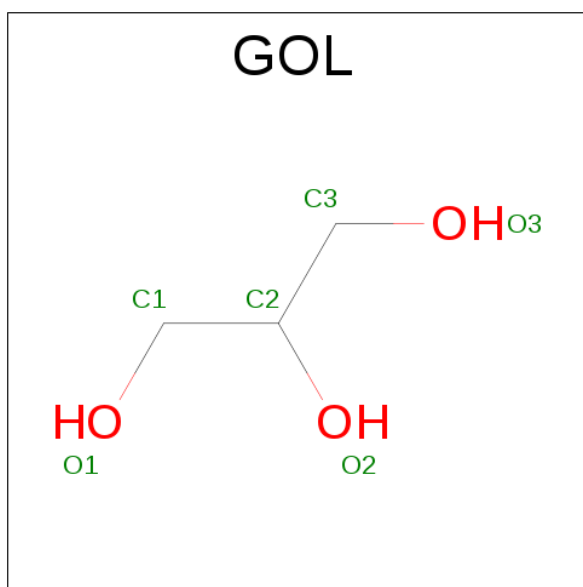
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	C	1	Total C O 5 3 2	0	0
3	C	1	Total C O 5 3 2	0	0
3	C	1	Total C O 5 3 2	0	0
3	D	1	Total C O 10 6 4	0	1
3	D	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	K	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	K	0	0
			2	2		

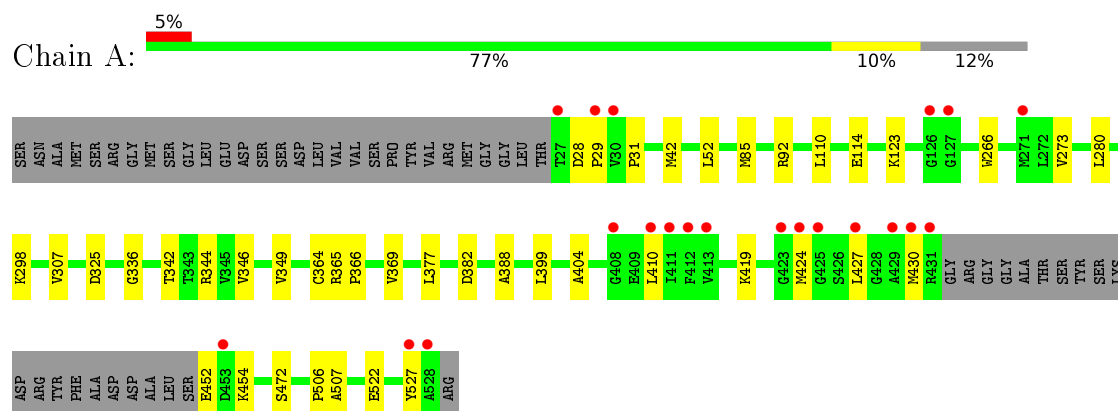
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	196	Total	O	0	0
			196	196		
6	B	204	Total	O	0	0
			204	204		
6	C	198	Total	O	0	0
			198	198		
6	D	195	Total	O	0	0
			195	195		

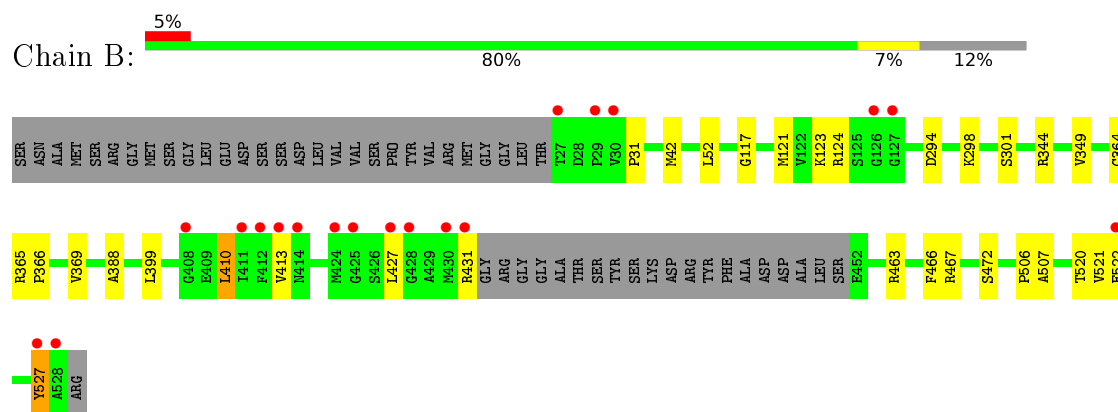
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

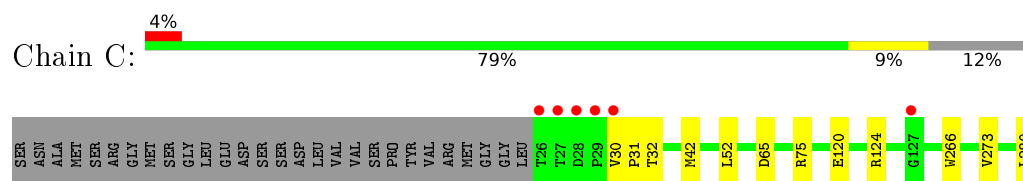
- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase

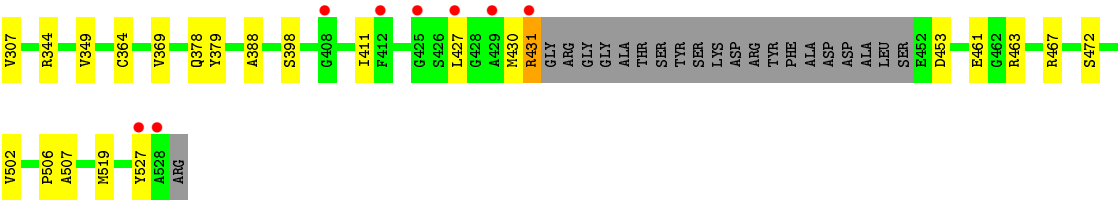


- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase

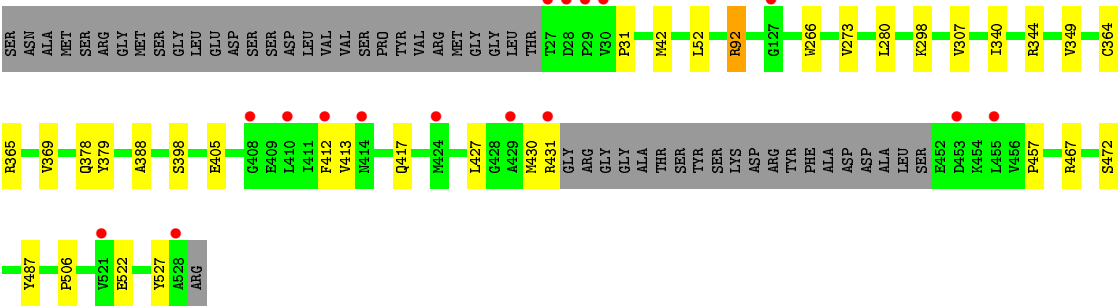
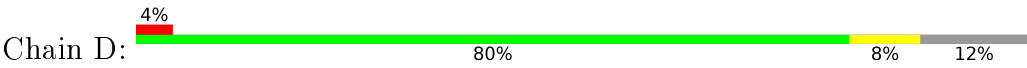


- Molecule 1: Inosine-5'-monophosphate dehydrogenase, Inosine-5'-monophosphate dehydrogenase





● Molecule 1: Inosine-5'-monophosphate dehydrogenase,Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.22Å 75.23Å 75.29Å 108.30° 108.25° 111.88°	Depositor
Resolution (Å)	35.73 – 1.69 35.73 – 1.69	Depositor EDS
% Data completeness (in resolution range)	91.2 (35.73-1.69) 76.7 (35.73-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.151 , 0.183 0.151 , 0.183	Depositor DCC
R_{free} test set	6426 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage

Continued on next page...

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.468 for $h+k+l, -l, -h$ 0.468 for $-l, h+k+l, -k$ 0.004 for $-l, -h, h+k+l$ 0.004 for $-k, h+k+l, -h$ 0.005 for $h+k+l, -h, -k$ 0.005 for $-k, -l, h+k+l$ 0.004 for $h, -h-k-l, k$ 0.004 for $h, l, -h-k-l$ 0.004 for $l, k, -h-k-l$ 0.004 for $-h-k-l, k, h$ 0.004 for k, l, h 0.004 for l, h, k 0.004 for $k, -h-k-l, l$ 0.004 for $-h-k-l, h, l$ 0.477 for $k, h, -h-k-l$ 0.024 for $-k, -h, -l$ 0.025 for $-h-k-l, l, k$ 0.005 for $h+k+l, -k, -l$ 0.024 for $l, -h-k-l, h$ 0.006 for $-h, h+k+l, -l$ 0.024 for $-h, -k, h+k+l$ 0.005 for $-h, -l, -k$ 0.006 for $-l, -k, -h$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11793	wwPDB-VP
Average B, all atoms (\AA^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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, K, PO4, PGO

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	0/2753	0.62	0/3734
1	B	0.49	0/2734	0.64	1/3713 (0.0%)
1	C	0.46	0/2764	0.61	0/3754
1	D	0.46	0/2738	0.61	0/3719
All	All	0.46	0/10989	0.62	1/14920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	TYR	CA-CB-CG	-5.15	103.61	113.40

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	2714	0	2771	36	0
1	B	2694	0	2754	33	0
1	C	2724	0	2782	31	0
1	D	2698	0	2761	33	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	32	2	0
3	B	20	0	32	8	0
3	C	15	0	24	11	0
3	D	25	0	40	25	0
4	A	24	0	32	4	0
4	B	12	0	16	6	0
4	C	18	0	24	3	0
4	D	12	0	16	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	196	0	0	4	0
6	B	204	0	0	2	0
6	C	198	0	0	6	0
6	D	195	0	0	4	0
All	All	11793	0	11284	139	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 6.

All (139) 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:B:527:TYR:CE1	4:B:604:GOL:H31	1.66	1.28
1:D:378:GLN:O	4:D:607:GOL:H31	1.45	1.15
1:B:527:TYR:HE1	4:B:604:GOL:C3	1.66	1.09
1:D:522:GLU:OE1	1:D:527:TYR:HD2	1.48	0.96
1:A:507:ALA:HB2	3:D:601[A]:PGO:H11	1.52	0.92
1:A:507:ALA:H	3:D:601[A]:PGO:H12	1.34	0.92
1:A:507:ALA:N	3:D:601[A]:PGO:H12	1.87	0.89
1:B:506:PRO:HG3	3:B:607:PGO:H32	1.56	0.86
1:B:527:TYR:HE1	4:B:604:GOL:H31	0.74	0.86
1:D:522:GLU:OE1	1:D:527:TYR:CD2	2.28	0.86
1:D:467:ARG:NH1	1:D:527:TYR:CE2	2.52	0.78
1:C:379:TYR:HA	3:C:607:PGO:H11	1.67	0.77
3:D:605:PGO:H32	3:D:606:PGO:O2	1.84	0.76
3:D:605:PGO:H12	3:D:606:PGO:O2	1.85	0.76
4:C:605:GOL:H32	6:C:729:HOH:O	1.86	0.76
1:B:506:PRO:CG	3:B:607:PGO:H32	2.16	0.75
1:A:507:ALA:CB	3:D:601[A]:PGO:H11	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:TYR:CD1	4:D:607:GOL:H32	2.24	0.73
3:B:607:PGO:H2	1:D:506:PRO:HB2	1.73	0.71
1:A:507:ALA:H	3:D:601[A]:PGO:C1	2.02	0.71
3:A:605:PGO:H2	6:A:764:HOH:O	1.89	0.70
1:D:378:GLN:O	4:D:607:GOL:C3	2.34	0.70
3:C:607:PGO:H12	6:C:833:HOH:O	1.94	0.66
1:B:507:ALA:CB	3:C:601:PGO:O1	2.44	0.66
1:C:506:PRO:HG3	3:C:601:PGO:O2	1.96	0.66
1:C:427:LEU:HA	1:C:430:MET:HE2	1.78	0.65
1:B:42:MET:HB2	1:C:31[B]:PRO:O	1.97	0.64
1:B:31[B]:PRO:O	1:D:42:MET:HB2	1.98	0.64
1:A:399:LEU:HD22	4:A:606:GOL:H11	1.80	0.63
1:A:85[B]:MET:SD	6:A:829:HOH:O	2.56	0.63
1:C:431:ARG:NH2	6:C:704:HOH:O	2.29	0.63
1:A:31[A]:PRO:O	1:C:42:MET:HB2	1.98	0.62
1:A:507:ALA:HB2	3:D:601[A]:PGO:C1	2.26	0.62
4:A:607:GOL:H31	1:C:507:ALA:HB2	1.80	0.62
1:B:506:PRO:HD2	3:C:601:PGO:H11	1.83	0.61
3:D:605:PGO:C3	3:D:606:PGO:O2	2.48	0.61
1:B:399:LEU:CD2	4:B:604:GOL:H11	2.32	0.59
1:D:506:PRO:CD	3:D:601[B]:PGO:H31	2.33	0.58
1:B:467:ARG:NH1	1:B:527:TYR:CE2	2.73	0.57
1:D:506:PRO:N	3:D:601[B]:PGO:H31	2.20	0.57
1:C:273:VAL:HG22	1:C:307[B]:VAL:HG21	1.86	0.57
1:C:378:GLN:O	3:C:607:PGO:H11	2.05	0.57
3:D:605:PGO:C3	3:D:606:PGO:H31	2.35	0.57
3:D:605:PGO:H33	3:D:606:PGO:C3	2.34	0.56
1:A:399:LEU:CD2	4:A:606:GOL:H11	2.35	0.56
1:B:507:ALA:HB2	3:C:601:PGO:O1	2.04	0.56
1:B:399:LEU:HD22	4:B:604:GOL:H11	1.88	0.56
1:A:85[B]:MET:SD	1:A:424:MET:HG2	2.45	0.55
1:D:365:ARG:NH2	6:D:701:HOH:O	2.25	0.55
1:D:92:ARG:HD2	1:D:405:GLU:HA	1.89	0.55
1:B:410:LEU:HD11	1:B:466:PHE:CD1	2.42	0.54
1:B:507:ALA:N	3:C:601:PGO:O1	2.38	0.54
1:D:506:PRO:HA	3:D:601[A]:PGO:H31	1.89	0.53
3:D:605:PGO:C3	3:D:606:PGO:C3	2.87	0.53
1:B:527:TYR:CE1	4:B:604:GOL:C3	2.57	0.53
1:C:266:TRP:CH2	1:C:298[A]:LYS:HG2	2.44	0.52
1:A:273:VAL:HG22	1:A:307[B]:VAL:HG21	1.92	0.52
1:D:506:PRO:CA	3:D:601[B]:PGO:H31	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HA	1:A:430:MET:HE2	1.91	0.51
1:A:42[B]:MET:HB2	1:D:31[B]:PRO:O	2.11	0.51
1:C:527:TYR:HE1	6:C:876:HOH:O	1.93	0.51
1:A:92[A]:ARG:NH2	1:A:404:ALA:O	2.44	0.50
1:D:506:PRO:CA	3:D:601[A]:PGO:H31	2.42	0.50
1:D:412[A]:PHE:CE1	1:D:417:GLN:HG2	2.47	0.49
1:C:453:ASP:OD2	6:C:701:HOH:O	2.20	0.49
1:D:506:PRO:HG3	3:D:601[B]:PGO:C3	2.43	0.49
1:A:266:TRP:CH2	1:A:298[A]:LYS:HG2	2.47	0.48
1:D:273:VAL:HG22	1:D:307[B]:VAL:HG21	1.95	0.48
1:D:427:LEU:HD13	1:D:457:PRO:HG3	1.96	0.48
1:A:507:ALA:HB2	3:D:601[B]:PGO:H11	1.95	0.48
1:A:42[B]:MET:HG3	1:C:502:VAL:HG23	1.96	0.47
1:D:472:SER:HB2	6:D:755:HOH:O	2.14	0.47
1:A:410:LEU:HD12	1:A:419:LYS:HD3	1.97	0.47
3:B:607:PGO:H2	1:D:506:PRO:CB	2.42	0.47
1:A:365:ARG:HB3	1:A:366:PRO:HD3	1.97	0.47
1:D:506:PRO:CG	3:D:601[B]:PGO:H31	2.44	0.47
1:C:75:ARG:HE	4:C:605:GOL:H2	1.78	0.47
1:B:364:CYS:HB3	1:B:369:VAL:O	2.15	0.47
1:A:507:ALA:CB	3:D:601[A]:PGO:C1	2.87	0.46
1:C:52:LEU:HD21	1:C:388:ALA:CB	2.46	0.46
1:A:110:LEU:HD12	1:A:114:GLU:HG2	1.98	0.46
1:C:379:TYR:CD1	3:C:607:PGO:H2	2.51	0.46
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.75	0.45
1:C:120:GLU:O	1:C:124:ARG:HG2	2.16	0.45
1:C:65:ASP:OD2	4:C:605:GOL:H32	2.15	0.45
3:D:605:PGO:H12	3:D:606:PGO:HO2	1.78	0.45
3:D:606:PGO:H2	6:D:837:HOH:O	2.16	0.45
1:C:364:CYS:HB3	1:C:369:VAL:O	2.16	0.45
1:C:467:ARG:HA	1:C:467:ARG:HD3	1.81	0.44
1:D:280:LEU:HG	1:D:307[B]:VAL:HG11	1.99	0.44
1:A:472:SER:HB2	6:A:754:HOH:O	2.16	0.44
1:A:452:GLU:HG2	1:A:454:LYS:H	1.81	0.44
1:D:344[A]:ARG:HG2	1:D:349[A]:VAL:O	2.17	0.44
1:B:52:LEU:HD21	1:B:388:ALA:CB	2.47	0.44
1:D:364:CYS:HB3	1:D:369:VAL:O	2.18	0.44
3:A:605:PGO:C2	6:A:764:HOH:O	2.56	0.44
1:B:294:ASP:O	1:B:298[B]:LYS:HG3	2.18	0.44
1:A:507:ALA:HB2	3:D:601[B]:PGO:C1	2.47	0.44
1:B:522:GLU:OE1	1:B:527:TYR:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:CYS:HB3	1:A:369:VAL:O	2.18	0.44
1:A:52:LEU:HD21	1:A:388:ALA:CB	2.48	0.43
1:B:365:ARG:HB3	1:B:366:PRO:HD3	2.00	0.43
3:D:605:PGO:H33	3:D:606:PGO:H33	2.00	0.43
1:C:472:SER:HB2	6:C:752:HOH:O	2.17	0.43
1:D:467:ARG:HG3	6:D:811:HOH:O	2.18	0.43
1:A:344[A]:ARG:HG2	1:A:349:VAL:O	2.17	0.43
1:A:377:LEU:HD23	1:A:382:ASP:HB3	2.01	0.43
1:B:117:GLY:O	1:B:121[A]:MET:HG3	2.19	0.43
1:A:522[B]:GLU:OE2	1:A:527:TYR:HA	2.18	0.43
1:B:123:LYS:HA	1:B:123:LYS:HD3	1.83	0.43
1:C:411:ILE:HD13	1:C:463[B]:ARG:HE	1.83	0.43
1:C:344[A]:ARG:HG2	1:C:349:VAL:O	2.18	0.43
1:C:519:MET:HB2	1:C:519:MET:HE2	1.88	0.42
1:B:506:PRO:CD	3:B:607:PGO:H32	2.49	0.42
1:B:521:VAL:HG12	1:C:461:GLU:HB2	2.02	0.42
1:A:280:LEU:HG	1:A:307[B]:VAL:HG11	2.02	0.42
1:B:344[A]:ARG:HG2	1:B:349[A]:VAL:O	2.19	0.42
1:C:280:LEU:HG	1:C:307[B]:VAL:HG11	2.02	0.42
1:D:266:TRP:CH2	1:D:298[A]:LYS:HG2	2.55	0.42
1:B:520:THR:HG21	1:C:463[B]:ARG:HG3	2.01	0.42
1:D:52:LEU:HD21	1:D:388:ALA:CB	2.49	0.41
1:A:336:GLY:HA3	1:A:344[A]:ARG:HG3	2.02	0.41
3:B:606:PGO:H2	1:D:487:TYR:CE2	2.55	0.41
1:B:298[A]:LYS:HE3	6:B:890:HOH:O	2.18	0.41
1:A:28[B]:ASP:HA	1:A:29[B]:PRO:HD3	1.84	0.41
1:B:472:SER:HB2	6:B:750:HOH:O	2.19	0.41
3:B:607:PGO:C2	1:D:506:PRO:HB2	2.46	0.41
1:A:123:LYS:HD2	1:A:123:LYS:HA	1.83	0.41
1:C:124:ARG:HD2	1:C:124:ARG:HA	1.91	0.41
1:C:30[B]:VAL:HG12	1:C:32[B]:THR:H	1.86	0.41
1:C:378:GLN:NE2	1:C:398[B]:SER:OG	2.52	0.41
1:A:342:THR:O	1:A:346:VAL:HG22	2.20	0.41
1:B:506:PRO:HG3	3:B:607:PGO:C3	2.39	0.41
1:D:379:TYR:HD1	4:D:607:GOL:H32	1.82	0.41
1:A:506:PRO:HG3	4:A:607:GOL:O2	2.20	0.41
1:D:467:ARG:HA	1:D:467:ARG:HD3	1.80	0.41
1:B:507:ALA:CB	3:C:601:PGO:HO1	2.34	0.40
1:C:379:TYR:CE1	3:C:607:PGO:H2	2.56	0.40
1:B:413:VAL:HG21	1:B:463[A]:ARG:NH1	2.37	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	373/407 (92%)	367 (98%)	6 (2%)	0	100	100
1	B	371/407 (91%)	365 (98%)	6 (2%)	0	100	100
1	C	375/407 (92%)	370 (99%)	5 (1%)	0	100	100
1	D	372/407 (91%)	366 (98%)	6 (2%)	0	100	100
All	All	1491/1628 (92%)	1468 (98%)	23 (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	281/300 (94%)	280 (100%)	1 (0%)	93	90
1	B	279/300 (93%)	273 (98%)	6 (2%)	60	39
1	C	283/300 (94%)	282 (100%)	1 (0%)	93	90
1	D	280/300 (93%)	274 (98%)	6 (2%)	61	42
All	All	1123/1200 (94%)	1109 (99%)	14 (1%)	78	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ASP
1	B	124	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	SER
1	B	410	LEU
1	B	427[A]	LEU
1	B	427[B]	LEU
1	B	431	ARG
1	C	431	ARG
1	D	92	ARG
1	D	340	ILE
1	D	398	SER
1	D	413	VAL
1	D	430	MET
1	D	431	ARG

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

Mol	Chain	Res	Type
1	A	118	GLN
1	B	378	GLN
1	C	378	GLN
1	C	498	GLN
1	D	118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	$\# Z > 2$
2	PO4	A	601	-	4,4,4	0.37	0	6,6,6	0.23	0
3	PGO	A	602	-	4,4,4	0.51	0	2,4,4	0.89	0
3	PGO	A	603	-	4,4,4	0.28	0	2,4,4	1.37	0
3	PGO	A	604	-	4,4,4	0.40	0	2,4,4	0.39	0
3	PGO	A	605	-	4,4,4	0.42	0	2,4,4	0.11	0
4	GOL	A	606	-	5,5,5	0.24	0	5,5,5	0.39	0
4	GOL	A	607	-	5,5,5	0.56	0	5,5,5	0.80	0
4	GOL	A	608	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	A	610	-	5,5,5	0.54	0	5,5,5	0.88	0
2	PO4	B	601	-	4,4,4	0.53	0	6,6,6	0.25	0
3	PGO	B	602	-	4,4,4	0.51	0	2,4,4	0.44	0
3	PGO	B	603	-	4,4,4	0.29	0	2,4,4	1.18	0
4	GOL	B	604	-	5,5,5	0.29	0	5,5,5	0.61	0
3	PGO	B	606	-	4,4,4	0.47	0	2,4,4	0.57	0
3	PGO	B	607	-	4,4,4	0.47	0	2,4,4	0.14	0
4	GOL	B	608	-	5,5,5	0.63	0	5,5,5	0.84	0
3	PGO	C	601	-	4,4,4	0.42	0	2,4,4	2.34	1 (50%)
2	PO4	C	602	-	4,4,4	0.63	0	6,6,6	0.22	0
3	PGO	C	603	-	4,4,4	0.47	0	2,4,4	0.73	0
4	GOL	C	604	-	5,5,5	0.43	0	5,5,5	0.36	0
4	GOL	C	605	-	5,5,5	0.21	0	5,5,5	0.27	0
4	GOL	C	606	-	5,5,5	0.18	0	5,5,5	0.53	0
3	PGO	C	607	-	4,4,4	0.18	0	2,4,4	0.39	0
3	PGO	D	601[A]	-	4,4,4	0.37	0	2,4,4	0.21	0
3	PGO	D	601[B]	-	4,4,4	0.23	0	2,4,4	2.25	1 (50%)
4	GOL	D	602	-	5,5,5	0.39	0	5,5,5	0.73	0
2	PO4	D	603	-	4,4,4	0.68	0	6,6,6	0.22	0
3	PGO	D	604	-	4,4,4	0.38	0	2,4,4	1.06	0
3	PGO	D	605	-	4,4,4	0.57	0	2,4,4	0.14	0
3	PGO	D	606	-	4,4,4	0.60	0	2,4,4	0.53	0
4	GOL	D	607	-	5,5,5	0.33	0	5,5,5	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	601	-	-	0/0/0/0	0/0/0/0
3	PGO	A	602	-	-	0/2/2/2	0/0/0/0
3	PGO	A	603	-	-	0/2/2/2	0/0/0/0
3	PGO	A	604	-	-	0/2/2/2	0/0/0/0
3	PGO	A	605	-	-	0/2/2/2	0/0/0/0
4	GOL	A	606	-	-	0/4/4/4	0/0/0/0
4	GOL	A	607	-	-	0/4/4/4	0/0/0/0
4	GOL	A	608	-	-	0/4/4/4	0/0/0/0
4	GOL	A	610	-	-	0/4/4/4	0/0/0/0
2	PO4	B	601	-	-	0/0/0/0	0/0/0/0
3	PGO	B	602	-	-	0/2/2/2	0/0/0/0
3	PGO	B	603	-	-	0/2/2/2	0/0/0/0
4	GOL	B	604	-	-	0/4/4/4	0/0/0/0
3	PGO	B	606	-	-	0/2/2/2	0/0/0/0
3	PGO	B	607	-	-	0/2/2/2	0/0/0/0
4	GOL	B	608	-	-	0/4/4/4	0/0/0/0
3	PGO	C	601	-	-	0/2/2/2	0/0/0/0
2	PO4	C	602	-	-	0/0/0/0	0/0/0/0
3	PGO	C	603	-	-	0/2/2/2	0/0/0/0
4	GOL	C	604	-	-	0/4/4/4	0/0/0/0
4	GOL	C	605	-	-	0/4/4/4	0/0/0/0
4	GOL	C	606	-	-	0/4/4/4	0/0/0/0
3	PGO	C	607	-	-	0/2/2/2	0/0/0/0
3	PGO	D	601[A]	-	-	0/2/2/2	0/0/0/0
3	PGO	D	601[B]	-	-	0/2/2/2	0/0/0/0
4	GOL	D	602	-	-	0/4/4/4	0/0/0/0
2	PO4	D	603	-	-	0/0/0/0	0/0/0/0
3	PGO	D	604	-	-	0/2/2/2	0/0/0/0
3	PGO	D	605	-	-	0/2/2/2	0/0/0/0
3	PGO	D	606	-	-	0/2/2/2	0/0/0/0
4	GOL	D	607	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	PGO	O1-C1-C2	-3.26	103.64	110.96
3	D	601[B]	PGO	O1-C1-C2	-3.11	103.97	110.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	PGO	2	0
4	A	606	GOL	2	0
4	A	607	GOL	2	0
4	B	604	GOL	6	0
3	B	606	PGO	1	0
3	B	607	PGO	7	0
3	C	601	PGO	6	0
4	C	605	GOL	3	0
3	C	607	PGO	5	0
3	D	601[A]	PGO	9	0
3	D	601[B]	PGO	7	0
3	D	605	PGO	8	0
3	D	606	PGO	9	0
4	D	607	GOL	4	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	357/407 (87%)	0.14	21 (5%)	26 27	17, 24, 54, 81	0
1	B	357/407 (87%)	0.11	19 (5%)	30 32	17, 24, 55, 88	0
1	C	358/407 (87%)	0.09	15 (4%)	40 44	17, 24, 55, 87	0
1	D	357/407 (87%)	0.12	16 (4%)	37 41	17, 24, 54, 78	0
All	All	1429/1628 (87%)	0.11	71 (4%)	32 35	17, 24, 55, 88	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	412[A]	PHE	7.7
1	A	412[A]	PHE	7.2
1	B	412[A]	PHE	7.1
1	B	431	ARG	6.6
1	A	27[B]	THR	6.5
1	C	412[A]	PHE	6.3
1	A	528	ALA	6.0
1	B	27[A]	THR	5.9
1	A	527	TYR	5.6
1	D	27[A]	THR	5.2
1	C	27[A]	THR	5.1
1	B	30[A]	VAL	4.8
1	C	30[A]	VAL	4.8
1	A	431	ARG	4.8
1	C	528	ALA	4.5
1	D	127	GLY	4.5
1	D	30[A]	VAL	4.3
1	C	26[A]	THR	4.2
1	B	29[A]	PRO	4.2
1	A	423	GLY	4.1
1	D	410	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	29[A]	PRO	3.9
1	B	528	ALA	3.9
1	A	30[A]	VAL	3.8
1	D	408	GLY	3.8
1	D	528	ALA	3.7
1	C	425	GLY	3.6
1	D	431	ARG	3.5
1	A	425	GLY	3.4
1	D	429	ALA	3.3
1	B	425	GLY	3.2
1	C	29[A]	PRO	3.1
1	B	127	GLY	2.9
1	A	410	LEU	2.9
1	A	430	MET	2.9
1	A	453	ASP	2.9
1	A	29[A]	PRO	2.8
1	A	413	VAL	2.8
1	D	414	ASN	2.8
1	A	126	GLY	2.7
1	D	521	VAL	2.7
1	A	411	ILE	2.6
1	D	28[A]	ASP	2.5
1	B	428	GLY	2.5
1	A	408	GLY	2.5
1	A	271[A]	MET	2.4
1	B	413	VAL	2.4
1	B	411	ILE	2.4
1	D	453	ASP	2.4
1	B	427[A]	LEU	2.4
1	C	28[A]	ASP	2.4
1	A	427	LEU	2.3
1	B	527	TYR	2.3
1	A	424	MET	2.3
1	B	126	GLY	2.3
1	C	431	ARG	2.3
1	A	127	GLY	2.3
1	B	430	MET	2.3
1	A	429	ALA	2.2
1	C	127	GLY	2.2
1	D	424	MET	2.2
1	B	408	GLY	2.2
1	C	527	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	305	ASP	2.1
1	C	427	LEU	2.1
1	C	429	ALA	2.1
1	C	408	GLY	2.1
1	B	522	GLU	2.1
1	B	414	ASN	2.1
1	B	424	MET	2.1
1	D	455	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	PGO	A	605	5/5	0.69	0.36	57.55	46,53,57,60	0
4	GOL	B	608	6/6	0.77	0.33	16.93	36,37,37,39	0
3	PGO	B	607	5/5	0.84	0.24	16.04	38,43,47,48	0
4	GOL	A	610	6/6	0.65	0.30	15.67	48,68,70,74	0
3	PGO	D	606	5/5	0.71	0.30	12.87	39,51,62,65	0
3	PGO	D	601[A]	5/5	0.80	0.25	11.44	35,41,44,48	5
3	PGO	D	601[B]	5/5	0.80	0.25	10.51	37,41,45,48	5
4	GOL	D	602	6/6	0.75	0.27	10.25	34,36,37,41	0
3	PGO	C	601	5/5	0.68	0.20	10.22	40,45,53,53	0
4	GOL	A	607	6/6	0.84	0.21	8.24	34,50,50,52	0
3	PGO	C	607	5/5	0.67	0.34	8.05	62,65,66,66	0
4	GOL	A	608	6/6	0.81	0.23	7.95	34,36,38,40	0
4	GOL	C	604	6/6	0.86	0.38	6.71	30,54,59,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	D	607	6/6	0.76	0.24	6.41	55,61,63,65	0
3	PGO	B	606	5/5	0.78	0.23	3.76	39,41,42,42	0
4	GOL	C	606	6/6	0.89	0.15	3.57	34,36,39,39	0
3	PGO	A	602	5/5	0.77	0.25	3.16	42,42,43,43	0
3	PGO	C	603	5/5	0.77	0.21	3.07	37,38,41,42	0
4	GOL	B	604	6/6	0.72	0.18	2.83	60,65,66,66	0
3	PGO	D	604	5/5	0.91	0.24	2.44	29,46,52,56	0
3	PGO	A	604	5/5	0.82	0.15	1.48	59,62,67,68	0
3	PGO	B	603	5/5	0.95	0.14	1.00	30,46,56,60	0
4	GOL	A	606	6/6	0.81	0.17	0.98	55,63,63,65	0
3	PGO	A	603	5/5	0.93	0.17	0.96	29,46,53,55	0
3	PGO	B	602	5/5	0.87	0.14	0.87	37,42,44,46	0
3	PGO	D	605	5/5	0.83	0.17	0.69	49,53,53,55	0
2	PO4	C	602	5/5	0.98	0.08	-0.07	17,19,21,22	0
2	PO4	D	603	5/5	0.98	0.08	-0.15	17,18,21,21	0
2	PO4	A	601	5/5	0.98	0.07	-0.76	17,19,22,22	0
2	PO4	B	601	5/5	0.99	0.05	-1.52	17,19,21,21	0
5	K	A	611	1/1	0.99	0.04	-2.68	20,20,20,20	0
5	K	B	609	1/1	0.98	0.04	-2.98	20,20,20,20	0
5	K	A	609	1/1	0.99	0.04	-4.15	20,20,20,20	0
5	K	B	605	1/1	0.99	0.03	-4.84	20,20,20,20	0
4	GOL	C	605	6/6	0.77	0.19	-	52,62,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.