



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:49 AM GMT

PDB ID : 3EZ3
Title : Crystal Structure of Plasmodium vivax geranylgeranylpyrophosphatesynthase PVX_092040 with zoledronate and IPP bound
Authors : Wernimont, A.K.; Lew, J.; Zhao, Y.; Kozieradzki, I.; Cossar, D.; Schapira, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)
Deposited on : 2008-10-22
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

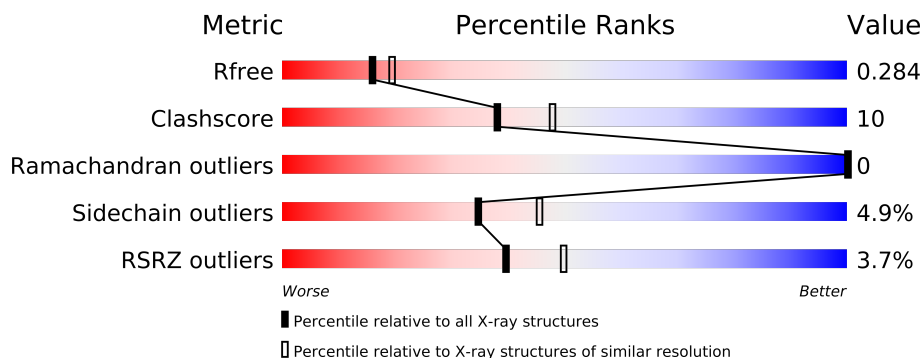
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	EDO	A	1105	-	X
5	EDO	B	1106	-	X
6	GOL	A	1106	-	X
6	GOL	B	1105	-	X
6	GOL	D	1105	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12384 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Farnesyl pyrophosphate synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	14	4	0
			2931	1909	465	541	16			
1	B	353	Total	C	N	O	S	11	3	0
			2910	1902	460	533	15			
1	C	357	Total	C	N	O	S	12	6	0
			2937	1917	467	538	15			
1	D	351	Total	C	N	O	S	14	4	0
			2887	1882	457	533	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5K4U6
A	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	SER	-	EXPRESSION TAG	UNP A5K4U6
A	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	SER	-	EXPRESSION TAG	UNP A5K4U6
A	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	21	GLY	-	EXPRESSION TAG	UNP A5K4U6

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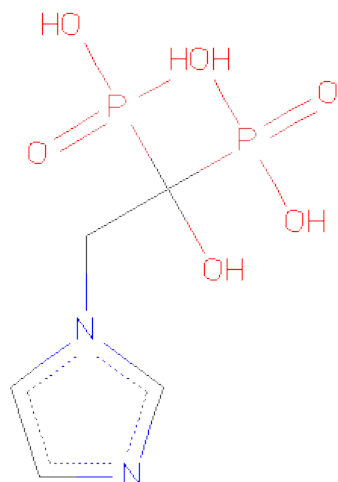
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	EXPRESSION TAG	UNP A5K4U6
B	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	SER	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	SER	-	EXPRESSION TAG	UNP A5K4U6
B	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	EXPRESSION TAG	UNP A5K4U6
C	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	SER	-	EXPRESSION TAG	UNP A5K4U6
C	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	SER	-	EXPRESSION TAG	UNP A5K4U6
C	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	17	LEU	-	EXPRESSION TAG	UNP A5K4U6

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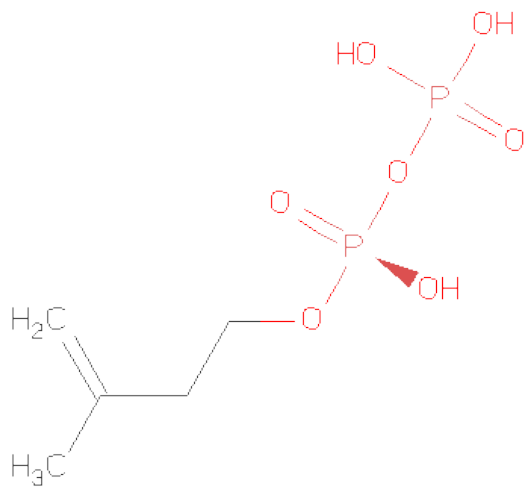
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
C	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	EXPRESSION TAG	UNP A5K4U6
D	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	SER	-	EXPRESSION TAG	UNP A5K4U6
D	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	SER	-	EXPRESSION TAG	UNP A5K4U6
D	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is ZOLEDRONIC ACID (three-letter code: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	B	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	C	1	Total	C	N	O	P	0	0
			16	5	2	7	2		
2	D	1	Total	C	N	O	P	0	0
			16	5	2	7	2		

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).

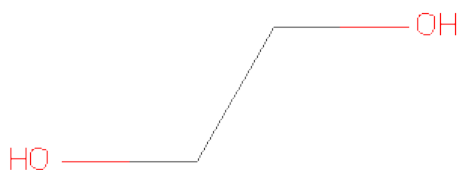


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			14	5	7	2		
3	B	1	Total	C	O	P	0	0
			14	5	7	2		
3	C	1	Total	C	O	P	0	0
			14	5	7	2		
3	D	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

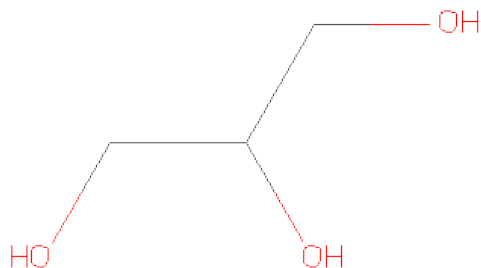
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Mg	0	0
			3	3		
4	A	3	Total	Mg	0	0
			3	3		
4	D	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

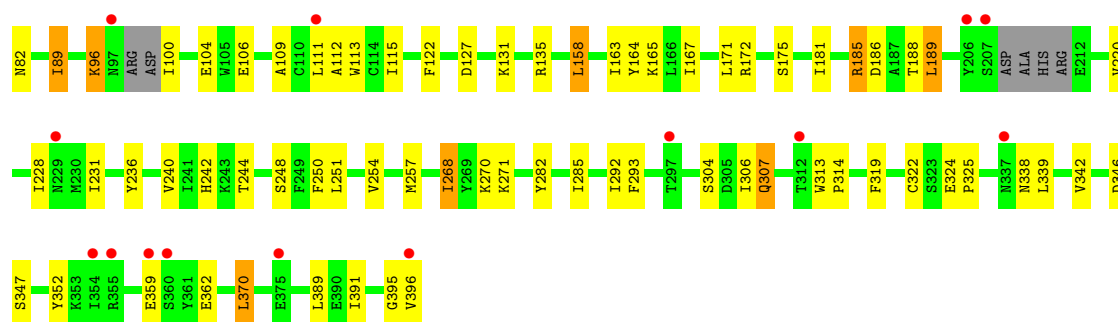
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

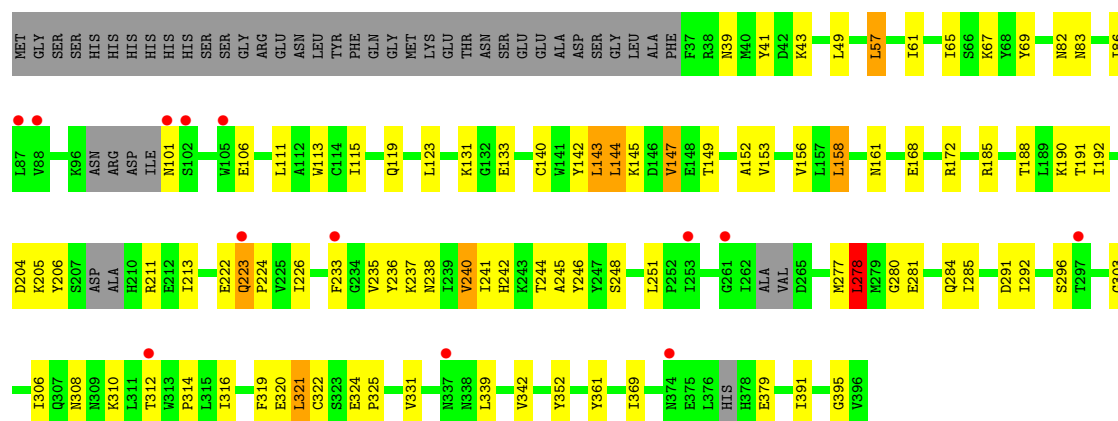
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	149	Total	O	0	0
			149	149		
7	B	140	Total	O	0	0
			140	140		
7	C	140	Total	O	0	0
			140	140		
7	D	132	Total	O	0	0
			132	132		



- Molecule 1: Farnesyl pyrophosphate synthase, putative

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.27Å 109.70Å 139.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.43 – 2.30 24.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.1 (24.43-2.30) 95.1 (24.43-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.291 0.222 , 0.284	Depositor DCC
R_{free} test set	3633 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	9 of 72250 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12384	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7001e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ZOL, EDO, IPE

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	0.76	5/3000 (0.2%)	0.78	5/4053 (0.1%)
1	B	0.79	2/2981 (0.1%)	0.90	7/4027 (0.2%)
1	C	1.30	6/3015 (0.2%)	1.12	9/4075 (0.2%)
1	D	0.73	1/2956 (0.0%)	0.81	4/3993 (0.1%)
All	All	0.92	14/11952 (0.1%)	0.91	25/16148 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	ARG	NE-CZ	-39.70	0.81	1.33
1	C	67	LYS	CD-CE	-31.96	0.71	1.51
1	C	59	GLU	CG-CD	-24.89	1.14	1.51
1	B	375	GLU	CG-CD	-14.97	1.29	1.51
1	C	60	GLU	CG-CD	-13.15	1.32	1.51
1	B	350	GLU	CD-OE2	-11.43	1.13	1.25
1	D	39	ASN	CA-CB	10.92	1.81	1.53
1	A	346	ASP	CG-OD2	-9.07	1.04	1.25
1	A	353	LYS	CG-CD	-8.97	1.22	1.52
1	C	307[A]	GLN	CD-OE1	-7.92	1.06	1.24
1	C	307[B]	GLN	CD-OE1	-7.92	1.06	1.24
1	A	368	LYS	CG-CD	-6.85	1.29	1.52
1	A	394	THR	CB-CG2	-6.67	1.30	1.52
1	A	356	LYS	CG-CD	-5.37	1.34	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	ARG	NE-CZ-NH2	-33.98	103.31	120.30
1	C	172	ARG	NE-CZ-NH1	33.04	136.82	120.30
1	B	350	GLU	CG-CD-OE1	-21.96	74.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	LYS	CG-CD-CE	17.05	163.06	111.90
1	B	350	GLU	OE1-CD-OE2	13.27	139.22	123.30
1	B	350	GLU	CG-CD-OE2	12.41	143.12	118.30
1	C	59	GLU	CB-CG-CD	8.98	138.44	114.20
1	C	59	GLU	CG-CD-OE2	8.97	136.23	118.30
1	C	59	GLU	CG-CD-OE1	-8.94	100.42	118.30
1	D	39	ASN	N-CA-CB	-7.51	97.08	110.60
1	D	39	ASN	CB-CA-C	-7.15	96.10	110.40
1	C	60	GLU	CB-CG-CD	7.05	133.23	114.20
1	B	155	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	171	LEU	CA-CB-CG	6.19	129.53	115.30
1	D	158	LEU	CA-CB-CG	-6.18	101.08	115.30
1	B	375	GLU	CB-CG-CD	5.92	130.18	114.20
1	A	45	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	135	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	158	LEU	CA-CB-CG	-5.57	102.49	115.30
1	C	158	LEU	CA-CB-CG	-5.37	102.95	115.30
1	D	278	LEU	CA-CB-CG	5.20	127.27	115.30
1	A	353	LYS	CB-CG-CD	5.06	124.75	111.60
1	A	45	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	158	LEU	CA-CB-CG	-5.03	103.72	115.30
1	B	288	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	2890	48	0
1	B	2910	0	2878	65	0
1	C	2937	0	2918	57	0
1	D	2887	0	2848	79	0
2	A	16	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	6	1	0
2	C	16	0	6	1	0
2	D	16	0	6	0	0
3	A	14	0	9	0	0
3	B	14	0	9	0	0
3	C	14	0	9	1	0
3	D	14	0	9	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	4	0
6	A	6	0	8	4	0
6	B	6	0	8	6	0
6	D	6	0	8	1	0
7	A	149	0	0	6	0
7	B	140	0	0	4	0
7	C	140	0	0	3	0
7	D	132	0	0	7	0
All	All	12384	0	11630	231	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (231) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:301:LYS:HG3	5:B:1106:EDO:H22	1.24	1.16
1:D:292:ILE:HD11	7:D:1164:HOH:O	1.46	1.15
1:D:241:ILE:HG23	1:D:277:MET:CE	1.77	1.15
1:A:126:ASP:OD1	7:A:1161:HOH:O	1.65	1.13
1:D:241:ILE:HG23	1:D:277:MET:HE1	1.43	1.00
1:D:241:ILE:HG23	1:D:277:MET:HE3	1.50	0.91
1:B:240:VAL:HG22	1:B:284:GLN:HG2	1.50	0.90
1:C:164:TYR:HB2	1:D:185[B]:ARG:HD3	1.52	0.89
1:C:164:TYR:CB	1:D:185[B]:ARG:HD3	2.05	0.87
1:B:244:THR:O	1:B:248:SER:HB2	1.76	0.85
1:D:240:VAL:HG22	1:D:284:GLN:HG2	1.58	0.83
1:A:143:LEU:HD13	6:A:1106:GOL:H32	1.61	0.83
1:B:296:SER:HB3	6:B:1105:GOL:H32	1.62	0.80
1:A:36:PHE:CE2	1:A:40[B]:MET:SD	2.75	0.80
1:C:304:SER:HA	1:C:307[B]:GLN:OE1	1.82	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:185[A]:ARG:HB2	1:C:185[A]:ARG:HH11	1.46	0.79
1:D:241:ILE:CG2	1:D:277:MET:HE3	2.14	0.76
1:D:233[B]:PHE:HE2	1:D:320:GLU:OE2	1.67	0.76
1:D:244:THR:O	1:D:248:SER:HB2	1.85	0.74
1:A:134:MET:HG2	7:A:1232:HOH:O	1.87	0.74
1:D:281:GLU:O	1:D:285:ILE:HG13	1.88	0.73
1:D:144:LEU:HB2	1:D:147:VAL:HG13	1.69	0.73
1:D:306:ILE:HD12	6:D:1105:GOL:H11	1.69	0.73
1:B:43:LYS:HE2	1:B:106:GLU:HG3	1.70	0.72
1:D:246:TYR:CE1	1:D:277:MET:HE1	2.25	0.72
1:A:58:GLU:HB2	1:A:61:ILE:HD12	1.72	0.71
1:B:233[B]:PHE:HE2	1:B:320:GLU:OE1	1.73	0.70
1:A:332:LYS:O	1:A:336:LYS:HE2	1.92	0.70
1:B:389:LEU:O	7:B:1192:HOH:O	2.10	0.69
1:A:168:GLU:OE2	1:B:185[A]:ARG:NH1	2.26	0.69
1:D:82:ASN:O	1:D:86:ILE:HG12	1.93	0.69
1:B:185[A]:ARG:NH2	1:B:186:ASP:OD1	2.26	0.68
1:B:340:ALA:O	1:B:344:VAL:HG23	1.94	0.68
1:A:164:TYR:OH	1:A:185[A]:ARG:HG3	1.93	0.67
1:C:96:LYS:HA	1:C:96:LYS:HE2	1.77	0.66
1:D:241:ILE:CG2	1:D:277:MET:CE	2.64	0.65
1:B:296:SER:HB3	6:B:1105:GOL:C3	2.28	0.64
1:D:246:TYR:CE1	1:D:277:MET:CE	2.80	0.64
1:A:164:TYR:CB	1:B:185[B]:ARG:HD3	2.28	0.64
1:A:143:LEU:CD1	6:A:1106:GOL:H32	2.26	0.63
1:B:245:ALA:HB2	1:B:280:GLY:HA3	1.81	0.62
1:B:250:PHE:O	1:B:254:VAL:HG23	1.99	0.62
1:B:89:ILE:HG23	1:B:105[A]:TRP:CZ3	2.34	0.62
1:C:257:MET:HE1	1:C:268:ILE:HG23	1.82	0.61
1:D:285:ILE:HD12	1:D:361:TYR:CZ	2.34	0.61
1:C:185[B]:ARG:NH2	1:C:186:ASP:OD1	2.34	0.61
1:A:241:ILE:HG23	1:A:277:MET:SD	2.42	0.60
1:B:301:LYS:HG3	5:B:1106:EDO:C2	2.17	0.60
1:C:164:TYR:HB3	1:D:185[B]:ARG:HD3	1.83	0.59
1:D:185[A]:ARG:NH2	7:D:1199:HOH:O	2.36	0.59
1:A:244:THR:O	1:A:248:SER:HB2	2.03	0.59
1:A:219[B]:ASN:H	1:A:219[B]:ASN:HD22	1.51	0.59
1:A:164:TYR:HB2	1:B:185[B]:ARG:HD3	1.83	0.59
1:C:89:ILE:HD12	1:C:112:ALA:HB2	1.84	0.58
1:B:101:ASN:O	1:B:105[B]:TRP:CE3	2.56	0.58
1:B:233[B]:PHE:HE1	1:B:313:TRP:CD1	2.21	0.58
1:D:43:LYS:HE2	1:D:106:GLU:HG3	1.84	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:ILE:O	1:C:167:ILE:HG13	2.04	0.57
1:D:223:GLN:HA	1:D:223:GLN:HE21	1.70	0.56
1:C:185[A]:ARG:HH11	1:C:185[A]:ARG:CB	2.18	0.56
1:B:303:GLY:N	6:B:1105:GOL:H12	2.21	0.56
1:D:320:GLU:HG2	1:D:321:LEU:HD13	1.87	0.55
7:A:1170:HOH:O	1:B:129:MET:CE	2.53	0.55
1:A:96:LYS:HA	1:A:96:LYS:HE2	1.88	0.55
1:A:236:TYR:HB2	1:A:316:ILE:CD1	2.37	0.55
1:A:343:LYS:HE3	1:C:346:ASP:OD1	2.05	0.55
1:A:226:ILE:HD11	1:A:331:VAL:HG22	1.87	0.55
2:B:397:ZOL:O16	5:B:1106:EDO:H11	2.07	0.55
1:B:338:ASN:HD21	1:D:133:GLU:CD	2.10	0.55
1:C:285:ILE:HG12	1:C:313:TRP:CD1	2.42	0.54
1:D:233[A]:PHE:CE2	1:D:237:LYS:HE2	2.43	0.54
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.42	0.54
1:B:342:VAL:HG23	1:D:339:LEU:HD13	1.88	0.54
1:D:152:ALA:O	1:D:156:VAL:HG23	2.08	0.54
1:C:127:ASP:OD2	1:C:135:ARG:HD2	2.08	0.53
1:B:233[B]:PHE:CE1	1:B:313:TRP:CD1	2.96	0.53
1:A:150[B]:LYS:HG2	1:A:151:ASN:N	2.24	0.53
1:D:149:THR:O	1:D:153:VAL:HG23	2.09	0.53
1:D:69:TYR:CD1	1:D:158:LEU:HD22	2.44	0.53
1:A:245:ALA:HB2	1:A:280:GLY:HA3	1.91	0.53
1:A:36:PHE:CZ	1:A:40[B]:MET:SD	3.01	0.53
1:C:307[B]:GLN:H	1:C:307[B]:GLN:CD	2.13	0.52
1:C:395:GLY:O	1:C:396:VAL:CB	2.58	0.52
1:C:40:MET:HE3	1:C:43:LYS:HG2	1.91	0.52
1:D:324[B]:GLU:HG3	1:D:325:PRO:HD3	1.90	0.52
1:D:140:CYS:HB2	1:D:143:LEU:HD22	1.92	0.52
1:A:119:GLN:NE2	1:A:123:LEU:HD21	2.25	0.51
1:B:233[B]:PHE:CE2	1:B:320:GLU:OE1	2.60	0.51
1:C:40:MET:CE	1:C:43:LYS:HG2	2.39	0.51
1:C:189[A]:LEU:HD13	1:D:161:ASN:HB3	1.91	0.51
1:A:236:TYR:CZ	1:A:240:VAL:HG11	2.46	0.51
1:B:303:GLY:HA2	5:B:1106:EDO:H21	1.91	0.51
1:A:327:LYS:O	1:A:331:VAL:HG23	2.11	0.51
1:C:370:LEU:HD13	1:C:389:LEU:HD23	1.93	0.51
1:B:249:PHE:O	1:B:253:ILE:HG13	2.10	0.51
1:D:240:VAL:CG1	1:D:281:GLU:HA	2.41	0.50
1:D:281:GLU:OE2	7:D:1267:HOH:O	2.19	0.50
1:A:164:TYR:HB3	1:B:185[B]:ARG:HD3	1.92	0.50
7:A:1170:HOH:O	1:B:129:MET:HE1	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:TYR:O	1:B:240:VAL:HB	2.12	0.50
1:C:236:TYR:CZ	1:C:240:VAL:HG11	2.47	0.50
1:C:370:LEU:HD13	1:C:389:LEU:CD2	2.41	0.50
1:C:46:ASP:O	1:C:50:SER:HB2	2.11	0.50
1:C:100:ILE:N	7:C:1209:HOH:O	2.45	0.50
1:D:278:LEU:HB3	1:D:369:ILE:HG12	1.94	0.49
1:C:244:THR:O	1:C:248:SER:HB2	2.12	0.49
1:A:125:ALA:O	1:A:129:MET:HG3	2.12	0.49
1:A:205:LYS:HG3	7:B:1225:HOH:O	2.13	0.49
1:B:303:GLY:H	6:B:1105:GOL:H12	1.76	0.49
1:C:36:PHE:O	1:C:40:MET:HG2	2.12	0.49
1:C:391:ILE:C	1:C:391:ILE:HD12	2.32	0.49
1:D:111:LEU:O	1:D:115:ILE:HG13	2.13	0.49
1:D:233[B]:PHE:CE2	1:D:320:GLU:OE2	2.57	0.49
1:A:205:LYS:HG2	1:A:213:ILE:HG13	1.95	0.49
1:B:91:ILE:HD12	1:B:384:VAL:HG11	1.94	0.49
1:B:91:ILE:O	1:B:95:VAL:HG23	2.13	0.49
1:D:245:ALA:HB2	1:D:280:GLY:HA3	1.94	0.49
1:D:235:VAL:O	1:D:238:ASN:HB2	2.13	0.49
1:D:240:VAL:HG22	1:D:284:GLN:CG	2.37	0.48
1:D:236:TYR:HB2	1:D:316:ILE:CD1	2.43	0.48
1:B:395:GLY:O	1:B:396:VAL:HG22	2.13	0.48
6:A:1106:GOL:H31	1:B:218:ILE:HD13	1.95	0.48
1:B:373:ILE:O	1:B:376:LEU:HB2	2.13	0.48
1:D:142:TYR:CZ	1:D:143:LEU:HD13	2.48	0.48
1:B:339:LEU:O	1:B:343:LYS:HB2	2.12	0.48
1:B:303:GLY:H	6:B:1105:GOL:H31	1.77	0.48
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.48	0.48
1:C:131:LYS:NZ	7:C:1140:HOH:O	2.37	0.48
1:C:135:ARG:NH2	2:C:397:ZOL:O15	2.30	0.47
1:A:119:GLN:NE2	1:A:123:LEU:CD2	2.77	0.47
1:A:195:GLN:NE2	7:A:1161:HOH:O	2.42	0.47
1:A:89:ILE:HD11	1:A:109:ALA:HA	1.95	0.47
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.50	0.47
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.49	0.47
1:B:240:VAL:HG22	1:B:284:GLN:CG	2.35	0.47
1:C:165:LYS:NZ	1:D:185[A]:ARG:HH11	2.11	0.47
1:A:72:LEU:O	1:A:76:ASN:HB2	2.14	0.47
7:A:1170:HOH:O	1:B:129:MET:HE3	2.15	0.47
1:D:69:TYR:CE1	1:D:158:LEU:HD22	2.49	0.47
1:A:133:GLU:CD	1:C:338:ASN:HD21	2.18	0.47
6:A:1106:GOL:H31	1:B:218:ILE:CD1	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:185[A]:ARG:HD2	1:D:161:ASN:OD1	2.14	0.46
1:D:115:ILE:HD13	1:D:251:LEU:HG	1.96	0.46
1:B:163:ILE:O	1:B:167:ILE:HG13	2.15	0.46
1:B:137:ASN:ND2	7:B:1173:HOH:O	2.28	0.46
1:A:185[A]:ARG:HG2	1:B:161:ASN:OD1	2.16	0.46
1:C:89:ILE:HD11	1:C:109:ALA:HA	1.97	0.46
1:C:338:ASN:O	1:C:342:VAL:HG13	2.16	0.46
1:D:205:LYS:HG3	1:D:206:TYR:CD2	2.51	0.46
1:B:236:TYR:CZ	1:B:240:VAL:HG21	2.51	0.46
1:A:244:THR:OG1	1:A:284:GLN:OE1	2.24	0.46
1:B:312:THR:HB	1:B:314:PRO:HD2	1.97	0.46
1:C:73:PHE:O	1:C:77:CYS:HB2	2.16	0.46
1:D:83:ASN:HB2	7:D:1218:HOH:O	2.15	0.45
1:A:199:THR:HG22	1:A:200:ASN:ND2	2.31	0.45
1:C:127:ASP:OD2	1:C:135:ARG:CD	2.65	0.45
1:A:98:ARG:O	1:A:100:ILE:N	2.50	0.45
1:D:61:ILE:O	1:D:65:ILE:HG12	2.17	0.45
1:B:205:LYS:HG3	1:B:206:TYR:CD2	2.51	0.45
1:B:339:LEU:HD21	1:D:342:VAL:HG11	1.99	0.45
1:D:226:ILE:HD11	1:D:331:VAL:HG22	1.99	0.45
1:C:40:MET:O	1:C:43:LYS:HB3	2.16	0.45
1:D:312:THR:HB	1:D:314:PRO:HD2	1.98	0.45
1:D:190:LYS:O	1:D:242:HIS:HB3	2.17	0.44
1:D:204:ASP:OD2	1:D:222:GLU:HG2	2.17	0.44
1:D:131:LYS:NZ	7:D:1156:HOH:O	2.48	0.44
1:C:282:TYR:OH	1:C:362:GLU:OE2	2.26	0.44
1:B:89:ILE:HD11	1:B:109:ALA:HA	1.99	0.44
1:B:81:LYS:HE3	7:B:1262:HOH:O	2.16	0.44
1:C:306:ILE:HB	1:C:307[B]:GLN:NE2	2.33	0.44
1:C:292:ILE:HG23	1:C:293:PHE:CE2	2.52	0.44
1:D:142:TYR:CE1	1:D:143:LEU:HD13	2.53	0.44
1:D:241:ILE:HD11	7:D:1267:HOH:O	2.18	0.43
1:D:222:GLU:O	1:D:224:PRO:HD3	2.18	0.43
1:B:387:TYR:O	1:B:391:ILE:HG13	2.18	0.43
1:B:296:SER:CB	6:B:1105:GOL:H32	2.40	0.43
1:C:185[B]:ARG:HH21	1:C:186:ASP:CG	2.21	0.43
1:B:152:ALA:O	1:B:156:VAL:HG23	2.18	0.43
1:C:135:ARG:HB3	7:C:1114:HOH:O	2.18	0.43
1:C:324:GLU:N	1:C:325:PRO:HD2	2.33	0.43
1:D:236:TYR:CZ	1:D:240:VAL:HG21	2.53	0.43
1:B:369:ILE:O	1:B:373:ILE:HG13	2.18	0.43
1:C:115:ILE:HD13	1:C:251:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:101:ASN:OD1	1:D:101:ASN:C	2.57	0.43
1:C:228:ILE:HA	1:C:231:ILE:HD12	2.01	0.43
1:D:190:LYS:HD3	1:D:246:TYR:CE1	2.54	0.43
1:D:233[A]:PHE:CD2	1:D:237:LYS:HE3	2.54	0.43
1:A:168:GLU:O	1:A:172:ARG:HG2	2.19	0.43
3:C:1101:IPE:H41	3:C:1101:IPE:H11	1.71	0.43
1:D:191:THR:HA	1:D:242:HIS:O	2.19	0.43
1:C:220:VAL:O	1:D:145:LYS:HG3	2.19	0.43
1:C:250:PHE:O	1:C:254:VAL:HG23	2.18	0.43
1:B:91:ILE:HG22	1:B:256:GLY:HA3	2.01	0.42
1:B:72:LEU:HD11	1:B:155:ASP:HB3	2.02	0.42
1:D:168:GLU:O	1:D:172:ARG:HG2	2.20	0.42
1:B:326:ASP:O	1:B:330:ILE:HG13	2.20	0.42
1:A:84:ARG:HB3	1:A:115:ILE:HG21	2.01	0.42
1:B:36:PHE:HZ	1:B:105[A]:TRP:HB3	1.85	0.42
1:D:119:GLN:NE2	1:D:123:LEU:HD11	2.35	0.42
1:D:233[A]:PHE:CE2	1:D:237:LYS:CE	3.03	0.42
1:D:133:GLU:OE2	7:D:1268:HOH:O	2.21	0.41
1:D:322:CYS:HA	1:D:352:TYR:CE1	2.55	0.41
1:C:270:LYS:HD2	1:C:270:LYS:HA	1.82	0.41
1:D:391:ILE:O	1:D:395:GLY:N	2.47	0.41
1:A:164:TYR:HH	1:A:185[A]:ARG:HG3	1.84	0.41
1:A:395:GLY:O	1:A:396:VAL:CB	2.67	0.41
1:A:193:ILE:HG13	1:B:55:TYR:CE2	2.55	0.41
1:D:291:ASP:OD2	1:D:303:GLY:HA2	2.21	0.41
1:C:69:TYR:O	1:C:73:PHE:HD2	2.04	0.41
1:A:286:HIS:O	1:A:289:TYR:HB3	2.21	0.41
1:B:273:GLU:O	1:B:277:MET:HG2	2.21	0.41
1:D:67:LYS:HB2	1:D:67:LYS:HE3	1.64	0.41
1:D:188:THR:HG22	1:D:192:ILE:HD11	2.01	0.41
1:B:235:VAL:O	1:B:238:ASN:HB2	2.20	0.41
1:A:185[A]:ARG:HD2	1:B:164:TYR:HB2	2.02	0.41
1:C:43:LYS:NZ	1:C:106:GLU:OE2	2.47	0.41
1:B:137:ASN:ND2	1:B:300:GLY:HA2	2.35	0.41
1:D:145:LYS:HD2	1:D:145:LYS:HA	1.80	0.41
1:A:204:ASP:OD2	1:A:222:GLU:HG3	2.21	0.41
1:D:285:ILE:HD12	1:D:361:TYR:OH	2.21	0.40
1:A:119:GLN:CD	1:A:123:LEU:HD22	2.41	0.40
1:C:242:HIS:CE1	1:D:57:LEU:HD13	2.56	0.40
1:D:308:ASN:HB3	1:D:310:LYS:HE2	2.03	0.40
1:C:322:CYS:HA	1:C:352:TYR:CE2	2.56	0.40
1:C:100:ILE:HA	1:C:104:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:236:TYR:HB2	1:D:316:ILE:HD11	2.02	0.40
1:B:36:PHE:CZ	1:B:105[A]:TRP:HB3	2.57	0.40
1:C:313:TRP:HB3	1:C:314:PRO:HD3	2.04	0.40
1:C:122:PHE:HZ	1:C:188:THR:HG23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	356/396 (90%)	349 (98%)	7 (2%)	0	100	100
1	B	348/396 (88%)	338 (97%)	10 (3%)	0	100	100
1	C	357/396 (90%)	347 (97%)	10 (3%)	0	100	100
1	D	345/396 (87%)	333 (96%)	12 (4%)	0	100	100
All	All	1406/1584 (89%)	1367 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	314/357 (88%)	301 (96%)	13 (4%)	41	55
1	B	312/357 (87%)	296 (95%)	16 (5%)	33	43
1	C	316/357 (88%)	297 (94%)	19 (6%)	27	35
1	D	309/357 (87%)	295 (96%)	14 (4%)	38	50
All	All	1251/1428 (88%)	1189 (95%)	62 (5%)	35	45

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	103	SER
1	A	111	LEU
1	A	115	ILE
1	A	123	LEU
1	A	134	MET
1	A	144	LEU
1	A	158	LEU
1	A	319	PHE
1	A	339	LEU
1	A	360	SER
1	A	363	LYS
1	A	370	LEU
1	B	36	PHE
1	B	50	SER
1	B	91	ILE
1	B	103	SER
1	B	111	LEU
1	B	138	LYS
1	B	165	LYS
1	B	189	LEU
1	B	193	ILE
1	B	198	ASP
1	B	241	ILE
1	B	278	LEU
1	B	319	PHE
1	B	356	LYS
1	B	371	SER
1	B	376	LEU
1	C	49	LEU
1	C	65	ILE
1	C	89	ILE
1	C	96	LYS
1	C	111	LEU
1	C	158	LEU
1	C	175	SER
1	C	181	ILE
1	C	185[A]	ARG
1	C	185[B]	ARG
1	C	189[A]	LEU
1	C	189[B]	LEU
1	C	268	ILE

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Mol	Chain	Res	Type
1	C	271	LYS
1	C	319	PHE
1	C	339	LEU
1	C	347	SER
1	C	359	GLU
1	C	370	LEU
1	D	49	LEU
1	D	57	LEU
1	D	143	LEU
1	D	144	LEU
1	D	147	VAL
1	D	211	ARG
1	D	213	ILE
1	D	223	GLN
1	D	240	VAL
1	D	278	LEU
1	D	296	SER
1	D	319	PHE
1	D	321	LEU
1	D	379	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	337	ASN
1	B	338	ASN
1	B	351	GLN
1	C	82	ASN
1	C	97	ASN
1	D	82	ASN
1	D	223	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	IPE	A	1101	-	13,13,13	1.90	3 (23%)	19,19,19	0.97	0
5	EDO	A	1105	-	3,3,3	0.65	0	2,2,2	0.15	0
6	GOL	A	1106	-	5,5,5	0.35	0	5,5,5	0.49	0
2	ZOL	A	397	4	16,16,16	3.01	11 (68%)	26,26,26	2.03	8 (30%)
3	IPE	B	1101	-	13,13,13	1.68	2 (15%)	19,19,19	1.41	3 (15%)
6	GOL	B	1105	-	5,5,5	0.41	0	5,5,5	0.80	0
5	EDO	B	1106	-	3,3,3	0.99	0	2,2,2	0.67	0
2	ZOL	B	397	4	16,16,16	2.89	8 (50%)	26,26,26	2.53	12 (46%)
3	IPE	C	1101	-	13,13,13	1.88	3 (23%)	19,19,19	1.70	6 (31%)
2	ZOL	C	397	4	16,16,16	2.39	9 (56%)	26,26,26	2.23	11 (42%)
3	IPE	D	1101	-	13,13,13	1.71	2 (15%)	19,19,19	1.11	1 (5%)
6	GOL	D	1105	-	5,5,5	0.39	0	5,5,5	0.42	0
2	ZOL	D	397	4	16,16,16	2.77	8 (50%)	26,26,26	2.28	10 (38%)

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	IPE	A	1101	-	-	0/13/13/13	0/0/0/0
5	EDO	A	1105	-	-	0/1/1/1	0/0/0/0
6	GOL	A	1106	-	-	0/4/4/4	0/0/0/0
2	ZOL	A	397	4	-	0/23/23/23	0/1/1/1
3	IPE	B	1101	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	1105	-	-	0/4/4/4	0/0/0/0
5	EDO	B	1106	-	-	0/1/1/1	0/0/0/0
2	ZOL	B	397	4	-	0/23/23/23	0/1/1/1
3	IPE	C	1101	-	-	0/13/13/13	0/0/0/0
2	ZOL	C	397	4	-	0/23/23/23	0/1/1/1
3	IPE	D	1101	-	-	0/13/13/13	0/0/0/0
6	GOL	D	1105	-	-	0/4/4/4	0/0/0/0
2	ZOL	D	397	4	-	0/23/23/23	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	ZOL	P9-O12	6.81	1.61	1.50
2	A	397	ZOL	P9-O12	5.97	1.60	1.50
2	D	397	ZOL	P14-O15	5.49	1.59	1.50
3	A	1101	IPE	C4-C3	5.32	1.51	1.33
3	C	1101	IPE	C4-C3	5.11	1.50	1.33
2	C	397	ZOL	P9-O12	5.07	1.58	1.50
3	D	1101	IPE	C4-C3	4.87	1.49	1.33
2	D	397	ZOL	P9-O12	4.79	1.58	1.50
3	B	1101	IPE	C4-C3	4.67	1.48	1.33
2	B	397	ZOL	P14-O15	4.42	1.57	1.50
2	D	397	ZOL	P9-O11	4.12	1.62	1.54
2	B	397	ZOL	P14-O16	4.01	1.62	1.54
2	A	397	ZOL	P14-O16	3.95	1.62	1.54
2	A	397	ZOL	P9-O10	-3.87	1.47	1.54
2	A	397	ZOL	P9-O11	3.87	1.62	1.54
2	C	397	ZOL	P14-O17	-3.87	1.47	1.54
2	A	397	ZOL	P14-O15	3.84	1.56	1.50
2	A	397	ZOL	P14-O17	-3.76	1.47	1.54
2	D	397	ZOL	P14-O16	3.63	1.61	1.54
2	C	397	ZOL	P14-C8	3.61	1.88	1.85
2	B	397	ZOL	O13-C8	-3.57	1.40	1.44
3	B	1101	IPE	C5-C3	-3.32	1.32	1.47
2	D	397	ZOL	P14-O17	-3.22	1.48	1.54
3	D	1101	IPE	C5-C3	-3.16	1.33	1.47
2	A	397	ZOL	O13-C8	-3.13	1.40	1.44
2	B	397	ZOL	C16-N15	-3.11	1.32	1.36
3	C	1101	IPE	C5-C3	-3.07	1.33	1.47
3	A	1101	IPE	C5-C3	-3.07	1.33	1.47
2	D	397	ZOL	C16-N15	-2.92	1.32	1.36
2	B	397	ZOL	P14-C8	-2.85	1.82	1.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	397	ZOL	P14-O15	2.83	1.55	1.50
2	B	397	ZOL	P9-O10	-2.81	1.49	1.54
2	A	397	ZOL	P14-C8	2.75	1.87	1.85
2	B	397	ZOL	P14-O17	-2.65	1.49	1.54
2	D	397	ZOL	P9-C8	2.61	1.87	1.85
2	C	397	ZOL	O13-C8	-2.55	1.41	1.44
2	C	397	ZOL	P9-O10	-2.36	1.50	1.54
2	A	397	ZOL	C19-N15	-2.25	1.33	1.37
2	A	397	ZOL	C16-N15	-2.23	1.33	1.36
2	C	397	ZOL	C19-N15	-2.21	1.33	1.37
2	C	397	ZOL	P14-O16	2.20	1.59	1.54
2	C	397	ZOL	C16-N15	-2.17	1.33	1.36
3	C	1101	IPE	PA-O3A	2.11	1.63	1.59
2	A	397	ZOL	P9-C8	-2.09	1.83	1.85
3	A	1101	IPE	PA-O3A	2.04	1.63	1.59
2	D	397	ZOL	P14-C8	2.02	1.86	1.85

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	ZOL	C8-C7-N15	5.07	115.17	110.90
2	D	397	ZOL	O16-P14-O15	-4.84	102.32	113.14
2	A	397	ZOL	C8-C7-N15	4.70	114.86	110.90
2	B	397	ZOL	C19-N15-C16	4.64	110.77	106.37
2	B	397	ZOL	C8-C7-N15	4.58	114.76	110.90
2	B	397	ZOL	P9-C8-C7	4.38	116.26	107.59
2	C	397	ZOL	C19-N15-C16	4.24	110.38	106.37
2	B	397	ZOL	O10-P9-C8	4.17	115.78	105.98
2	D	397	ZOL	N17-C16-N15	-4.17	104.95	111.96
2	B	397	ZOL	N17-C16-N15	-4.13	105.00	111.96
2	D	397	ZOL	O11-P9-O12	-4.08	104.03	113.14
2	A	397	ZOL	O17-P14-C8	3.78	114.86	105.98
2	C	397	ZOL	P9-C8-P14	-3.63	106.35	112.78
2	B	397	ZOL	P9-C8-P14	-3.59	106.43	112.78
2	D	397	ZOL	P9-C8-C7	3.56	114.64	107.59
2	A	397	ZOL	C19-N15-C16	3.56	109.74	106.37
2	B	397	ZOL	O17-P14-C8	3.54	114.30	105.98
2	D	397	ZOL	C19-N15-C16	3.34	109.53	106.37
2	A	397	ZOL	O10-P9-C8	3.08	113.20	105.98
3	C	1101	IPE	O1-PA-O1A	-3.01	97.59	109.37
3	C	1101	IPE	PA-O1-C1	3.00	138.55	121.66
3	C	1101	IPE	O2A-PA-O1	2.98	123.53	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	ZOL	O10-P9-C8	2.90	112.80	105.98
2	B	397	ZOL	O12-P9-C8	-2.89	102.44	110.04
2	D	397	ZOL	O16-P14-O17	2.89	116.17	107.93
3	B	1101	IPE	O3B-PB-O2B	2.85	119.76	110.44
2	C	397	ZOL	N17-C16-N15	-2.81	107.23	111.96
2	C	397	ZOL	O17-P14-C8	2.81	112.58	105.98
2	A	397	ZOL	O17-P14-O15	2.79	119.39	113.14
2	A	397	ZOL	N17-C16-N15	-2.79	107.27	111.96
2	C	397	ZOL	O11-P9-O12	-2.72	107.07	113.14
2	C	397	ZOL	O10-P9-O12	-2.62	107.29	113.14
3	B	1101	IPE	O2A-PA-O3A	2.49	116.94	105.14
2	B	397	ZOL	O16-P14-O17	2.45	114.92	107.93
3	C	1101	IPE	O3A-PA-O1	-2.42	92.58	103.41
2	D	397	ZOL	C8-C7-N15	2.42	112.94	110.90
2	A	397	ZOL	O15-P14-C8	-2.40	103.74	110.04
3	C	1101	IPE	O3B-PB-O1B	2.40	116.94	107.61
2	D	397	ZOL	O11-P9-O10	2.38	114.70	107.93
2	C	397	ZOL	O16-P14-C8	-2.26	100.66	105.98
2	A	397	ZOL	P14-C8-C7	2.25	112.03	107.59
2	C	397	ZOL	O11-P9-O10	2.22	114.26	107.93
2	D	397	ZOL	P9-C8-P14	-2.22	108.86	112.78
3	B	1101	IPE	C5-C3-C2	2.17	123.33	114.98
3	C	1101	IPE	O2A-PA-O3A	2.16	115.40	105.14
2	B	397	ZOL	O15-P14-C8	-2.11	104.50	110.04
3	D	1101	IPE	O3B-PB-O1B	2.06	115.64	107.61
2	B	397	ZOL	O10-P9-O12	-2.04	108.57	113.14
2	C	397	ZOL	O12-P9-C8	-2.03	104.70	110.04
2	B	397	ZOL	O16-P14-C8	-2.01	101.26	105.98
2	D	397	ZOL	C18-C19-N15	2.00	108.15	106.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	358/396 (90%)	0.21	12 (3%)	43 53	16, 24, 32, 49	18 (5%)
1	B	353/396 (89%)	0.18	10 (2%)	50 60	18, 24, 31, 48	15 (4%)
1	C	357/396 (90%)	0.22	16 (4%)	32 42	17, 24, 32, 46	12 (3%)
1	D	351/396 (88%)	0.19	13 (3%)	39 50	17, 24, 32, 52	7 (1%)
All	All	1419/1584 (89%)	0.20	51 (3%)	39 51	16, 24, 32, 52	52 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	PHE	5.9
1	B	105[A]	TRP	5.5
1	A	35	ALA	4.6
1	C	207	SER	4.5
1	B	377	HIS	4.0
1	C	35	ALA	3.9
1	A	207	SER	3.8
1	A	312	THR	3.6
1	C	111	LEU	3.5
1	A	98	ARG	3.3
1	B	87	LEU	3.1
1	A	355	ARG	3.0
1	B	396	VAL	2.9
1	A	111	LEU	2.9
1	D	297	THR	2.8
1	D	223	GLN	2.8
1	D	101	ASN	2.8
1	C	312	THR	2.8
1	B	253	ILE	2.7
1	D	261	GLY	2.7
1	A	101	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	355	ARG	2.6
1	B	88	VAL	2.6
1	D	88	VAL	2.5
1	C	359	GLU	2.5
1	A	36	PHE	2.5
1	C	97	ASN	2.4
1	D	312	THR	2.4
1	C	337	ASN	2.4
1	D	253	ILE	2.4
1	A	315	LEU	2.3
1	D	87	LEU	2.3
1	C	354	ILE	2.3
1	C	36	PHE	2.3
1	A	325	PRO	2.3
1	B	297	THR	2.2
1	D	337	ASN	2.2
1	C	206	TYR	2.2
1	D	105	TRP	2.2
1	A	102	SER	2.2
1	D	374	ASN	2.2
1	C	297	THR	2.2
1	D	102	SER	2.2
1	B	383	TYR	2.2
1	C	375	GLU	2.1
1	C	360	SER	2.1
1	C	396	VAL	2.1
1	A	229	ASN	2.1
1	B	39	ASN	2.1
1	D	233[A]	PHE	2.0
1	C	229	ASN	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EDO	B	1106	4/4	0.41	16.31	25,25,25,26	0
6	GOL	A	1106	6/6	0.43	9.45	50,52,53,53	0
6	GOL	D	1105	6/6	0.28	5.52	36,41,42,43	0
6	GOL	B	1105	6/6	0.26	4.53	32,36,37,38	0
5	EDO	A	1105	4/4	0.29	3.92	47,50,51,51	0
4	MG	A	1103	1/1	0.13	-0.14	18,18,18,18	0
4	MG	B	1103	1/1	0.11	-0.31	10,10,10,10	0
4	MG	A	1104	1/1	0.13	-0.35	12,12,12,12	0
4	MG	C	1103	1/1	0.13	-0.45	17,17,17,17	0
4	MG	D	1103	1/1	0.10	-0.48	12,12,12,12	0
4	MG	C	1104	1/1	0.13	-0.62	16,16,16,16	0
2	ZOL	A	397	16/16	0.11	-0.73	11,15,19,20	0
2	ZOL	C	397	16/16	0.12	-0.75	10,13,18,19	0
2	ZOL	B	397	16/16	0.10	-0.83	11,14,17,19	0
3	IPE	C	1101	14/14	0.11	-1.18	2,15,19,20	3
3	IPE	D	1101	14/14	0.08	-1.42	9,16,20,21	0
4	MG	B	1102	1/1	0.09	-1.45	12,12,12,12	0
3	IPE	B	1101	14/14	0.08	-1.56	12,14,16,17	0
4	MG	B	1104	1/1	0.06	-1.79	6,6,6,6	0
4	MG	D	1102	1/1	0.08	-1.93	9,9,9,9	0
2	ZOL	D	397	16/16	0.08	-2.03	7,12,17,17	0
3	IPE	A	1101	14/14	0.07	-2.09	14,16,18,19	0
4	MG	A	1102	1/1	0.03	-3.44	9,9,9,9	0
4	MG	D	1104	1/1	0.06	-4.48	8,8,8,8	0
4	MG	C	1102	1/1	0.05	-16.04	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.