Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:38 AM BST

PDB ID	:	6MH5
Title	:	Crystal Structure of 1-deoxy-D-xylulose-5-phosphate reductoisomerase from Staphylococcus schleiferi in complex with Fosmidomycin (FOM)
Authors	:	Lee, S.G.; Jez, J.M.
Deposited on	:	2018-09-17
Resolution	:	2.89 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 ⓘ symbol.

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

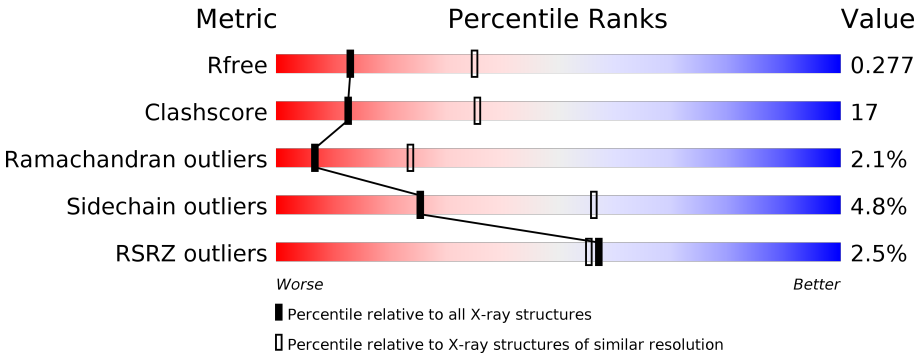
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 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	376	3% 63% 34%
1	B	376	2% 63% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FOM	B	701	-	X	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5920 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.

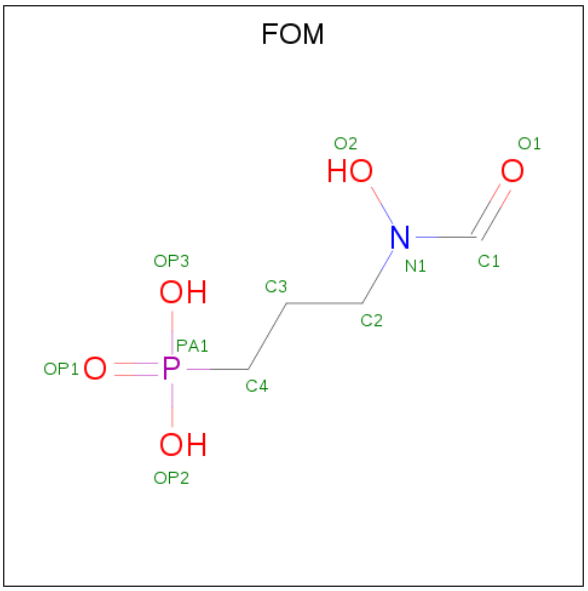
- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2942	1874	494	558	16			
1	B	375	Total	C	N	O	S	0	0	0
			2956	1882	498	560	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	GLU	conflict	UNP A0A0K1A7V6
A	284	VAL	ALA	conflict	UNP A0A0K1A7V6
A	349	SER	ALA	conflict	UNP A0A0K1A7V6
A	367	HIS	TYR	conflict	UNP A0A0K1A7V6
B	188	GLY	GLU	conflict	UNP A0A0K1A7V6
B	284	VAL	ALA	conflict	UNP A0A0K1A7V6
B	349	SER	ALA	conflict	UNP A0A0K1A7V6
B	367	HIS	TYR	conflict	UNP A0A0K1A7V6

- Molecule 2 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (three-letter code: FOM) (formula: $C_4H_{10}NO_5P$).



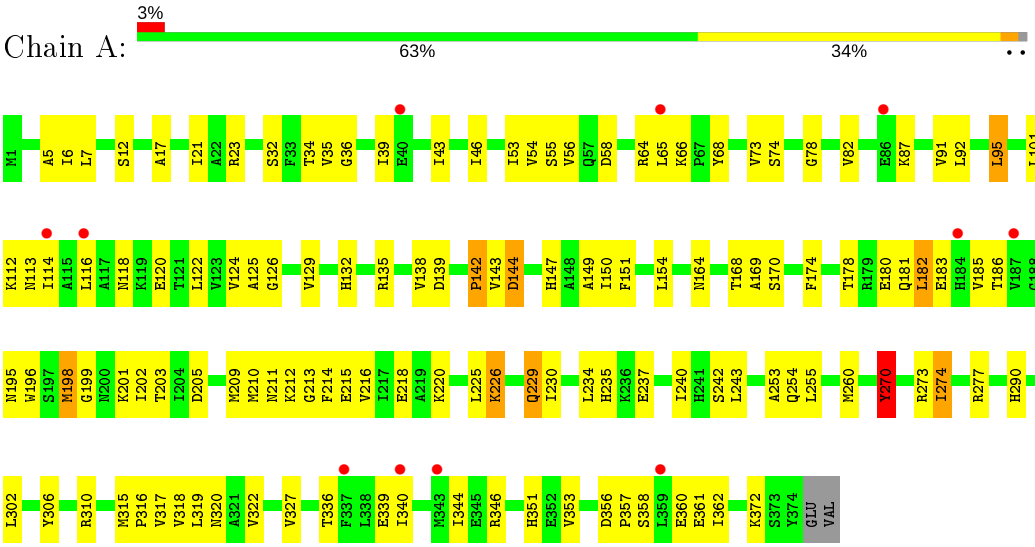
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			11	4	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			11	4	1	5	1		

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.

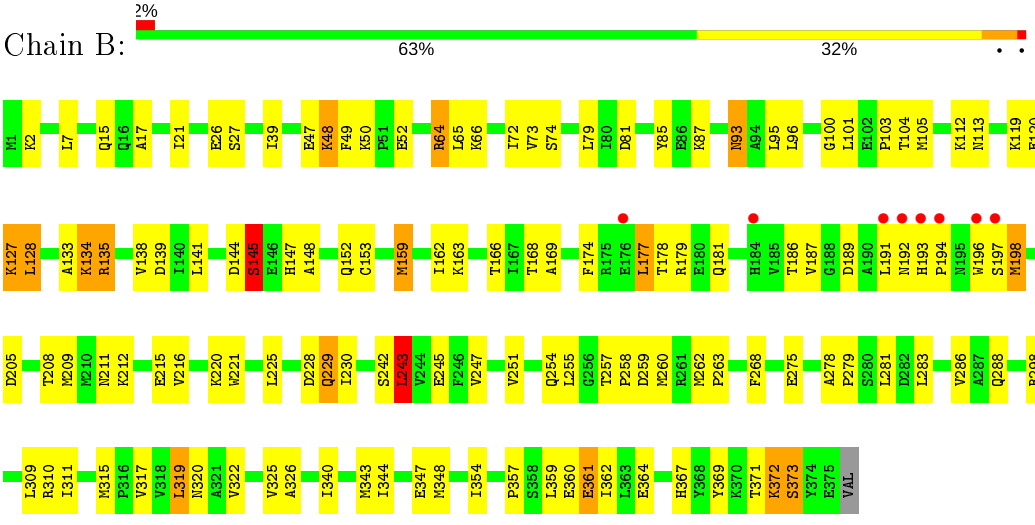
- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain A:



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.71Å 53.98Å 115.80Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	46.08 – 2.89 46.08 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.4 (46.08-2.89) 97.4 (46.08-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.212 , 0.277 0.212 , 0.277	Depositor DCC
R_{free} test set	1818 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	66.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5920	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: FOM

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	0.46	0/2997	0.64	1/4056 (0.0%)
1	B	0.51	1/3011 (0.0%)	0.67	4/4073 (0.1%)
All	All	0.49	1/6008 (0.0%)	0.65	5/8129 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	ASN	C-N	7.10	1.50	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	LEU	CA-CB-CG	8.66	135.21	115.30
1	B	243	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	95	LEU	CA-CB-CG	6.16	129.47	115.30
1	B	319	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	153	CYS	CA-CB-SG	5.16	123.30	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	ALA	Peptide

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	2942	0	2955	95	0
1	B	2956	0	2972	102	0
2	A	11	0	8	1	0
2	B	11	0	8	1	0
All	All	5920	0	5943	197	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 17.

All (197) 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:2:LYS:NZ	1:B:268:PHE:O	2.07	0.87
1:B:212:LYS:NZ	2:B:701:FOM:OP2	2.09	0.86
1:A:169:ALA:HA	1:A:212:LYS:HE3	1.62	0.80
1:A:32:SER:HB2	1:A:82:VAL:HG23	1.64	0.80
1:B:193:HIS:HB2	1:B:203:THR:HG23	1.66	0.77
1:B:39:ILE:HG21	1:B:64:ARG:HG2	1.67	0.77
1:A:168:THR:HG21	1:A:240:ILE:O	1.90	0.71
1:A:358:SER:OG	1:A:361:GLU:OE1	2.07	0.71
1:A:151:PHE:HE1	1:A:270:TYR:CE1	2.08	0.70
1:B:347:GLU:OE1	1:B:372:LYS:NZ	2.21	0.69
1:B:113:ASN:ND2	1:B:139:ASP:OD2	2.26	0.68
1:A:199:GLY:HA3	1:A:203:THR:HG23	1.77	0.66
1:A:322:VAL:HG11	1:A:344:ILE:HA	1.77	0.66
1:B:168:THR:O	1:B:212:LYS:HE2	1.95	0.65
1:A:7:LEU:HA	1:A:34:THR:HB	1.77	0.65
1:A:73:VAL:HG12	1:A:74:SER:H	1.62	0.65
1:B:105:MET:HE2	1:B:128:LEU:HD13	1.78	0.65
1:B:120:GLU:HG2	1:B:320:ASN:OD1	1.96	0.65
1:A:178:THR:HG22	1:A:181:GLN:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:THR:N	1:B:181:GLN:OE1	2.22	0.65
1:B:7:LEU:HB2	1:B:93:ASN:HA	1.79	0.64
1:B:65:LEU:HB3	1:B:72:ILE:HD13	1.80	0.63
1:A:186:THR:HG23	1:A:189:ASP:H	1.63	0.63
1:B:174:PHE:HB3	1:B:177:LEU:HD22	1.79	0.63
1:B:126:GLY:O	1:B:127:LYS:HB3	1.99	0.62
1:B:119:LYS:HD3	1:B:215:GLU:HG3	1.80	0.62
1:A:151:PHE:CE1	1:A:270:TYR:CE1	2.86	0.62
1:B:85:TYR:O	1:B:112:LYS:HE3	2.00	0.62
1:B:220:LYS:HD2	1:B:309:LEU:HD11	1.80	0.62
1:A:243:LEU:HD13	1:A:253:ALA:HB2	1.81	0.61
1:B:193:HIS:CD2	1:B:196:TRP:H	2.17	0.61
1:A:35:VAL:HG22	1:A:36:GLY:O	1.99	0.61
1:A:296:LEU:HD21	1:A:302:LEU:HD23	1.83	0.61
1:B:127:LYS:HB2	1:B:221:TRP:CZ3	2.35	0.61
1:A:226:LYS:HD2	1:A:226:LYS:N	2.16	0.60
1:B:257:THR:O	1:B:259:ASP:N	2.34	0.60
1:B:174:PHE:O	1:B:298:ARG:NH2	2.29	0.60
1:B:159:MET:HG3	1:B:162:ILE:HD11	1.85	0.59
1:B:166:THR:HB	1:B:243:LEU:HD23	1.85	0.58
1:B:147:HIS:HE1	1:B:215:GLU:HB3	1.67	0.58
1:B:216:VAL:HG13	1:B:230:ILE:HG21	1.85	0.58
1:A:306:TYR:O	1:A:310:ARG:HG3	2.03	0.58
1:A:143:VAL:O	1:A:144:ASP:HB2	2.04	0.57
1:B:119:LYS:NZ	1:B:211:ASN:OD1	2.37	0.57
1:A:201:LYS:NZ	1:A:205:ASP:OD1	2.37	0.57
1:A:56:VAL:HG12	1:A:74:SER:HB3	1.87	0.56
1:B:186:THR:HG23	1:B:189:ASP:H	1.70	0.56
1:A:46:ILE:HD11	1:A:54:VAL:HG21	1.86	0.56
1:B:120:GLU:O	1:B:124:VAL:HG22	2.04	0.56
1:B:262:MET:HB3	1:B:263:PRO:HD3	1.88	0.56
1:B:319:LEU:CD1	1:B:348:MET:HE1	2.36	0.56
1:B:340:ILE:O	1:B:344:ILE:HG13	2.06	0.56
1:A:322:VAL:HG12	1:A:344:ILE:HG12	1.88	0.55
1:A:357:PRO:HB2	1:A:362:ILE:HG13	1.88	0.55
1:B:93:ASN:ND2	1:B:95:LEU:H	2.04	0.55
1:A:240:ILE:HG12	1:A:255:LEU:HG	1.89	0.55
1:A:199:GLY:O	1:A:203:THR:N	2.21	0.55
1:A:43:ILE:HD11	1:A:64:ARG:HD2	1.90	0.54
1:A:211:ASN:O	1:A:215:GLU:HG3	2.07	0.54
1:A:212:LYS:O	1:A:216:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD12	1:A:95:LEU:O	2.08	0.54
1:B:208:THR:HG22	1:B:301:CYS:SG	2.47	0.54
1:A:180:GLU:OE2	1:A:180:GLU:N	2.40	0.54
1:B:319:LEU:HD12	1:B:348:MET:HE1	1.89	0.54
1:A:169:ALA:HA	1:A:212:LYS:CE	2.36	0.53
1:A:23:ARG:NH2	1:A:277:ARG:O	2.42	0.53
1:B:361:GLU:HA	1:B:364:GLU:HB2	1.91	0.53
1:B:260:MET:O	1:B:263:PRO:HD2	2.09	0.53
1:A:124:VAL:HG13	1:A:317:VAL:HG22	1.91	0.52
1:B:148:ALA:O	1:B:152:GLN:HG3	2.09	0.52
1:A:105:MET:SD	1:A:129:VAL:HG12	2.50	0.52
1:B:113:ASN:HA	1:B:138:VAL:HG13	1.92	0.52
1:B:93:ASN:HD22	1:B:95:LEU:H	1.56	0.52
1:A:339:GLU:HA	1:A:339:GLU:OE1	2.10	0.52
1:B:93:ASN:HD21	1:B:95:LEU:HB2	1.75	0.52
1:B:124:VAL:HG12	1:B:317:VAL:HA	1.92	0.51
1:B:101:LEU:HD22	1:B:359:LEU:HD11	1.93	0.51
1:B:357:PRO:HB2	1:B:362:ILE:HG13	1.91	0.51
1:A:73:VAL:HG12	1:A:74:SER:N	2.26	0.51
1:A:270:TYR:C	1:A:270:TYR:CD1	2.84	0.51
1:A:201:LYS:HD2	1:A:327:VAL:HG11	1.92	0.51
1:B:225:LEU:HB2	1:B:230:ILE:HD11	1.91	0.50
1:B:354:ILE:HB	1:B:357:PRO:HG3	1.94	0.50
1:B:105:MET:HE2	1:B:128:LEU:CD1	2.40	0.50
1:B:159:MET:O	1:B:162:ILE:HG13	2.10	0.50
1:A:182:LEU:HA	1:A:185:VAL:HG13	1.94	0.50
1:A:209:MET:HG2	1:A:302:LEU:HD13	1.93	0.50
1:A:318:VAL:HG21	1:A:351:HIS:CG	2.47	0.49
1:A:336:THR:O	1:A:339:GLU:HB2	2.12	0.49
1:A:212:LYS:HE2	2:A:701:FOM:OP1	2.12	0.49
1:A:124:VAL:HG13	1:A:317:VAL:HG13	1.95	0.49
1:A:104:THR:HG23	1:A:114:ILE:HG21	1.95	0.48
1:A:112:LYS:O	1:A:138:VAL:HG21	2.13	0.48
1:A:12:SER:HB3	1:A:198:MET:HE3	1.94	0.48
1:A:360:GLU:OE2	1:A:360:GLU:N	2.39	0.48
1:B:100:GLY:O	1:B:103:PRO:HD2	2.14	0.48
1:B:322:VAL:O	1:B:325:VAL:HG12	2.14	0.48
1:B:147:HIS:HE1	1:B:215:GLU:CB	2.27	0.48
1:A:132:HIS:HA	1:A:135:ARG:HB2	1.96	0.48
1:A:151:PHE:HE1	1:A:270:TYR:CD1	2.32	0.48
1:B:245:GLU:HB2	1:B:251:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:O	1:B:288:GLN:N	2.44	0.47
1:A:213:GLY:O	1:A:216:VAL:HG22	2.13	0.47
1:A:237:GLU:OE2	1:A:290:HIS:N	2.41	0.47
1:B:101:LEU:HD12	1:B:124:VAL:CG2	2.45	0.47
1:A:178:THR:O	1:A:182:LEU:HD12	2.15	0.47
1:B:47:GLU:O	1:B:47:GLU:HG2	2.15	0.47
1:A:149:ALA:HB3	1:A:242:SER:HB3	1.96	0.47
1:B:201:LYS:NZ	1:B:205:ASP:OD2	2.33	0.47
1:B:367:HIS:O	1:B:371:THR:HG23	2.14	0.47
1:A:64:ARG:O	1:A:64:ARG:HD3	2.15	0.47
1:B:144:ASP:O	1:B:147:HIS:N	2.43	0.46
1:B:360:GLU:H	1:B:360:GLU:CD	2.16	0.46
1:B:361:GLU:H	1:B:361:GLU:HG2	1.56	0.46
1:A:220:LYS:HE2	1:A:225:LEU:O	2.15	0.46
1:A:39:ILE:CG1	1:A:65:LEU:HD11	2.46	0.46
1:A:113:ASN:HA	1:A:138:VAL:CG2	2.46	0.46
1:B:344:ILE:HG22	1:B:348:MET:HE3	1.97	0.46
1:A:273:ARG:O	1:A:274:ILE:HG12	2.16	0.46
1:A:118:ASN:OD1	1:A:120:GLU:HB2	2.16	0.46
1:A:174:PHE:CG	1:A:182:LEU:HD21	2.51	0.45
1:B:198:MET:HG2	1:B:202:ILE:HG21	1.98	0.45
1:B:347:GLU:HB3	1:B:369:TYR:HE1	1.80	0.45
1:A:195:ASN:HB2	1:A:203:THR:HG22	1.99	0.45
1:B:101:LEU:HD12	1:B:124:VAL:HG23	1.99	0.45
1:B:186:THR:OG1	1:B:187:VAL:N	2.50	0.45
1:B:326:ALA:HB2	1:B:343:MET:HE2	1.98	0.45
1:B:73:VAL:HG11	1:B:81:ASP:OD2	2.17	0.45
1:A:214:PHE:O	1:A:218:GLU:HG3	2.16	0.45
1:B:306:TYR:O	1:B:310:ARG:HG2	2.17	0.45
1:A:43:ILE:HG12	1:A:68:TYR:CD2	2.51	0.44
1:B:163:LYS:HG3	1:B:247:VAL:HA	1.98	0.44
1:B:163:LYS:HG3	1:B:247:VAL:HG12	1.99	0.44
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.71	0.44
1:A:340:ILE:O	1:A:344:ILE:HG13	2.17	0.44
1:A:234:LEU:HG	1:A:294:MET:HE1	2.00	0.44
1:B:100:GLY:O	1:B:104:THR:HG23	2.18	0.44
1:B:159:MET:HG3	1:B:162:ILE:CD1	2.47	0.44
1:A:235:HIS:CE1	1:A:237:GLU:HB2	2.52	0.44
1:A:5:ALA:HB3	1:A:91:VAL:HG22	1.99	0.44
1:B:147:HIS:CE1	1:B:215:GLU:HB3	2.51	0.44
1:B:93:ASN:C	1:B:93:ASN:HD22	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LYS:O	1:B:135:ARG:HB2	2.17	0.43
1:B:101:LEU:CD2	1:B:359:LEU:HD11	2.47	0.43
1:B:242:SER:O	1:B:243:LEU:HB3	2.18	0.43
1:A:199:GLY:HA2	1:A:202:ILE:HB	2.00	0.43
1:B:281:LEU:HG	1:B:283:LEU:HD12	1.99	0.43
1:B:319:LEU:HD12	1:B:348:MET:CE	2.48	0.43
1:A:122:LEU:CD2	1:A:126:GLY:HA2	2.48	0.43
1:A:150:ILE:O	1:A:154:LEU:HG	2.18	0.43
1:B:26:GLU:HG2	1:B:27:SER:N	2.33	0.43
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.70	0.43
1:B:254:GLN:C	1:B:255:LEU:HD12	2.39	0.43
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.59	0.43
1:B:50:LYS:N	1:B:50:LYS:HD2	2.33	0.43
1:A:39:ILE:HA	1:A:39:ILE:HD12	1.91	0.43
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.70	0.43
1:B:17:ALA:O	1:B:21:ILE:HG13	2.19	0.42
1:B:311:ILE:HG21	1:B:315:MET:HE2	2.00	0.42
1:A:120:GLU:HG3	1:A:320:ASN:OD1	2.19	0.42
1:B:196:TRP:HD1	1:B:198:MET:CE	2.32	0.42
1:B:127:LYS:HB2	1:B:221:TRP:CH2	2.54	0.42
1:B:198:MET:HG3	1:B:198:MET:O	2.19	0.42
1:A:17:ALA:O	1:A:21:ILE:HG13	2.20	0.42
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.62	0.42
1:B:52:GLU:OE2	1:B:87:LYS:HE3	2.19	0.42
1:B:278:ALA:HB1	1:B:279:PRO:HD2	2.01	0.42
1:A:35:VAL:O	1:A:56:VAL:HA	2.19	0.42
1:A:180:GLU:O	1:A:183:GLU:HG3	2.19	0.42
1:A:182:LEU:HD23	1:A:185:VAL:HG11	2.01	0.42
1:A:193:HIS:CD2	1:A:194:PRO:HD2	2.54	0.42
1:B:197:SER:HA	1:B:198:MET:HB3	2.02	0.42
1:B:225:LEU:HB3	1:B:229:GLN:HB3	2.01	0.42
1:B:73:VAL:HG12	1:B:74:SER:H	1.84	0.42
1:A:315:MET:N	1:A:316:PRO:HD2	2.34	0.42
1:B:212:LYS:HA	1:B:212:LYS:HD3	1.81	0.41
1:A:32:SER:HB3	1:A:53:ILE:HG22	2.01	0.41
1:B:281:LEU:HD21	1:B:283:LEU:HD11	2.01	0.41
1:B:48:LYS:HG2	1:B:49:PHE:CE2	2.54	0.41
1:B:166:THR:HB	1:B:243:LEU:CD2	2.50	0.41
1:A:210:MET:SD	1:A:319:LEU:HD21	2.61	0.41
1:A:225:LEU:HD22	1:A:229:GLN:NE2	2.36	0.41
1:A:142:PRO:HB2	1:A:147:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:MET:HE3	1:A:209:MET:HB2	1.88	0.41
1:B:209:MET:HE2	1:B:209:MET:HB2	1.97	0.41
1:A:54:VAL:HG12	1:A:55:SER:N	2.36	0.41
1:A:73:VAL:CG1	1:A:78:GLY:HA2	2.51	0.41
1:A:101:LEU:HD21	1:A:125:ALA:HB3	2.03	0.41
1:A:182:LEU:O	1:A:185:VAL:HG22	2.21	0.41
1:A:6:ILE:HG12	1:A:92:LEU:HD23	2.03	0.41
1:B:169:ALA:HB2	1:B:212:LYS:HG3	2.03	0.41
1:A:199:GLY:O	1:A:202:ILE:N	2.54	0.41
1:A:32:SER:HB3	1:A:53:ILE:CG2	2.51	0.40
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.87	0.40
1:A:113:ASN:HA	1:A:138:VAL:HG23	2.03	0.40
1:B:144:ASP:O	1:B:145:SER:C	2.59	0.40
1:B:372:LYS:HG2	1:B:373:SER:N	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	372/376 (99%)	345 (93%)	18 (5%)	9 (2%)	6 20
1	B	373/376 (99%)	339 (91%)	27 (7%)	7 (2%)	8 26
All	All	745/752 (99%)	684 (92%)	45 (6%)	16 (2%)	7 24

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASP
1	A	270	TYR
1	A	274	ILE
1	B	48	LYS

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Mol	Chain	Res	Type
1	A	198	MET
1	A	229	GLN
1	A	372	LYS
1	B	127	LYS
1	B	135	ARG
1	B	194	PRO
1	B	198	MET
1	B	258	PRO
1	A	142	PRO
1	B	145	SER
1	A	230	ILE
1	A	353	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/327 (99%)	310 (96%)	14 (4%)	29	60
1	B	326/327 (100%)	309 (95%)	17 (5%)	23	53
All	All	650/654 (99%)	619 (95%)	31 (5%)	25	56

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	66	LYS
1	A	87	LYS
1	A	139	ASP
1	A	164	ASN
1	A	170	SER
1	A	182	LEU
1	A	196	TRP
1	A	226	LYS
1	A	254	GLN
1	A	260	MET

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Mol	Chain	Res	Type
1	A	270	TYR
1	A	346	ARG
1	A	356	ASP
1	B	15	GLN
1	B	64	ARG
1	B	66	LYS
1	B	93	ASN
1	B	96	LEU
1	B	128	LEU
1	B	134	LYS
1	B	145	SER
1	B	159	MET
1	B	179	ARG
1	B	228	ASP
1	B	229	GLN
1	B	243	LEU
1	B	275	GLU
1	B	361	GLU
1	B	372	LYS
1	B	373	SER

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	164	ASN
1	A	229	GLN
1	B	93	ASN
1	B	132	HIS
1	B	155	ASN
1	B	193	HIS
1	B	195	ASN
1	B	367	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	FOM	A	701	-	9,10,10	5.10	2 (22%)	11,13,13	3.74	6 (54%)
2	FOM	B	701	-	9,10,10	4.65	2 (22%)	11,13,13	4.47	8 (72%)

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	FOM	A	701	-	-	4/7/9/9	-
2	FOM	B	701	-	-	3/7/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FOM	PA1-C4	-12.87	1.66	1.78
2	B	701	FOM	PA1-C4	-11.95	1.67	1.78
2	A	701	FOM	C1-N1	7.91	1.46	1.34
2	B	701	FOM	C1-N1	6.62	1.44	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FOM	PA1-C4-C3	7.85	124.81	114.98
2	A	701	FOM	OP3-PA1-C4	-7.71	88.81	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FOM	OP3-PA1-C4	-7.60	89.07	106.95
2	A	701	FOM	OP2-PA1-C4	6.82	123.00	106.95
2	B	701	FOM	OP3-PA1-OP1	-5.49	97.88	112.39
2	B	701	FOM	OP2-PA1-C4	4.95	118.61	106.95
2	B	701	FOM	OP1-PA1-C4	4.05	118.89	111.40
2	B	701	FOM	O2-N1-C2	3.89	123.24	113.67
2	A	701	FOM	OP3-PA1-OP1	-3.65	102.73	112.39
2	A	701	FOM	O2-N1-C2	3.19	121.52	113.67
2	A	701	FOM	OP2-PA1-OP1	3.05	120.46	112.39
2	A	701	FOM	OP3-PA1-OP2	-2.89	99.63	108.08
2	B	701	FOM	O1-C1-N1	-2.24	119.35	125.80
2	B	701	FOM	OP2-PA1-OP1	2.22	118.27	112.39

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FOM	C3-C2-N1-O2
2	A	701	FOM	C2-C3-C4-PA1
2	A	701	FOM	C3-C4-PA1-OP1
2	B	701	FOM	C2-C3-C4-PA1
2	B	701	FOM	C3-C4-PA1-OP2
2	A	701	FOM	N1-C2-C3-C4
2	B	701	FOM	C3-C4-PA1-OP3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FOM	1	0
2	B	701	FOM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	374/376 (99%)	0.30	11 (2%) 51 48	55, 68, 86, 93	0
1	B	375/376 (99%)	0.20	8 (2%) 63 62	54, 58, 74, 100	0
All	All	749/752 (99%)	0.25	19 (2%) 57 55	54, 61, 84, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	TRP	4.3
1	B	176	GLU	3.8
1	B	192	ASN	3.5
1	B	193	HIS	3.1
1	B	184	HIS	3.0
1	A	184	HIS	2.8
1	A	114	ILE	2.6
1	B	191	LEU	2.6
1	B	197	SER	2.5
1	A	65	LEU	2.4
1	A	40	GLU	2.4
1	A	359	LEU	2.4
1	A	116	LEU	2.2
1	A	86	GLU	2.1
1	B	194	PRO	2.1
1	A	340	ILE	2.1
1	A	337	PHE	2.0
1	A	343	MET	2.0
1	A	187	VAL	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	FOM	B	701	11/11	0.92	0.23	58,60,62,65	0
2	FOM	A	701	11/11	0.94	0.20	66,68,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.