Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:20 PM GMT

PDB ID	:	1JVS
Title	:	Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase; a target enzyme for antimalarial drugs
Authors	:	Yajima, S.; Nonaka, T.; Kuzuyama, T.; Seto, H.; Ohsawa, K.
Deposited on	:	2001-08-31
Resolution	:	2.20 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:

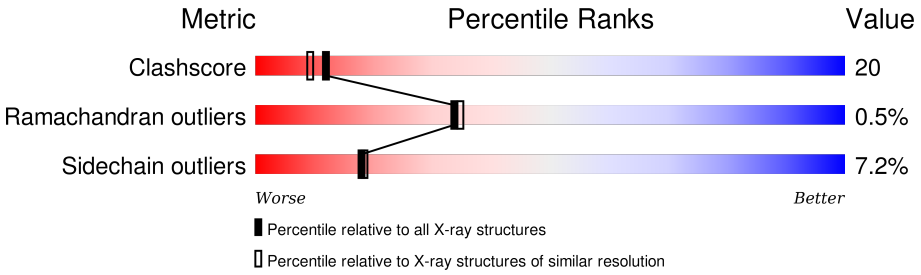
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	61% 34% 5%
1	B	400	66% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6446 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	400	Total	C	N	O	S	Se	0	0	0
			3037	1895	536	580	8	18			
1	B	398	Total	C	N	O	S	Se	0	0	0
			3025	1889	534	576	8	18			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	CLONING ARTIFACT	UNP P45568
A	41	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	55	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	67	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	87	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	97	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	135	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	200	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	213	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	224	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	225	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	245	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	258	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	275	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	283	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	321	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	366	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	368	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	393	MSE	MET	MODIFIED RESIDUE	UNP P45568
A	398	SER	-	CLONING ARTIFACT	UNP P45568
A	399	ALA	-	CLONING ARTIFACT	UNP P45568
B	0	GLY	-	CLONING ARTIFACT	UNP P45568
B	41	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	55	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	67	MSE	MET	MODIFIED RESIDUE	UNP P45568

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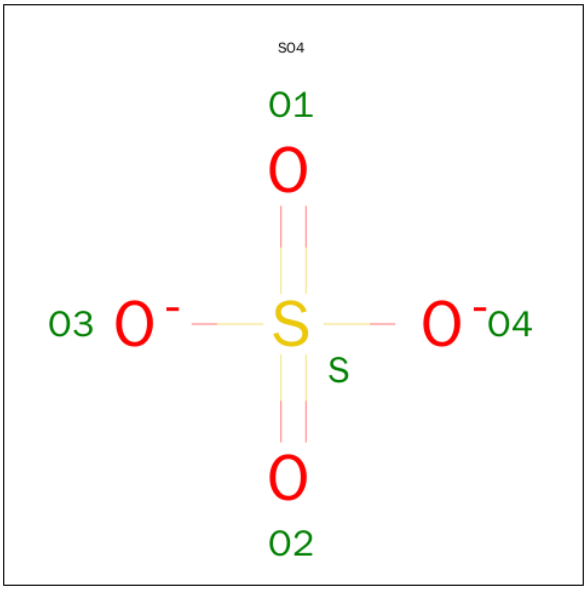
Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	97	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	135	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	200	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	213	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	224	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	225	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	245	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	258	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	275	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	283	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	321	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	366	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	368	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	393	MSE	MET	MODIFIED RESIDUE	UNP P45568
B	398	SER	-	CLONING ARTIFACT	UNP P45568
B	399	ALA	-	CLONING ARTIFACT	UNP P45568

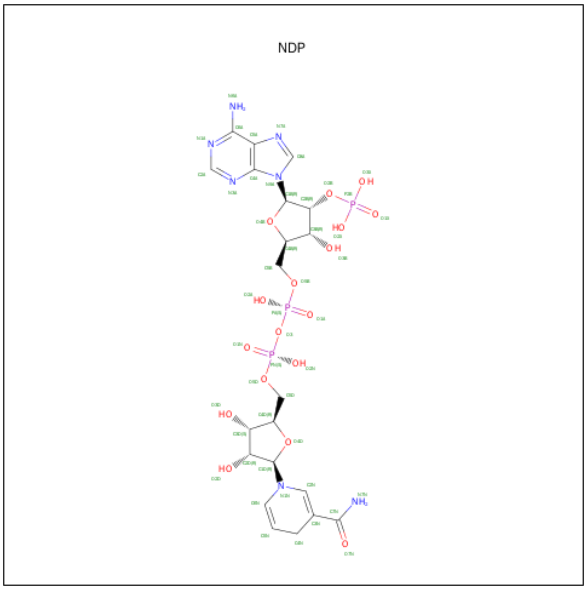
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	130	Total	O	0	0
			130	130		

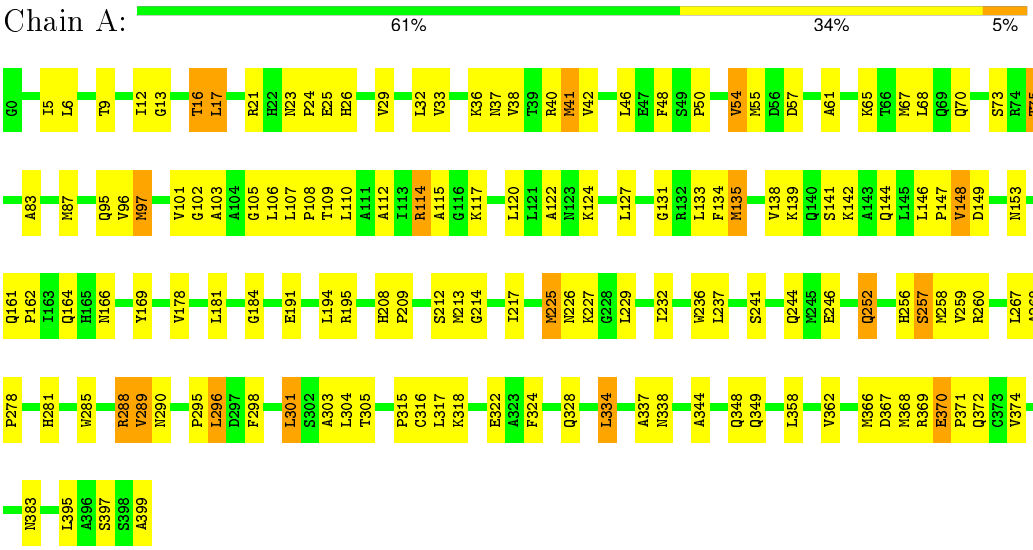
3 Residue-property plots (i)

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.

Note EDS was not executed.

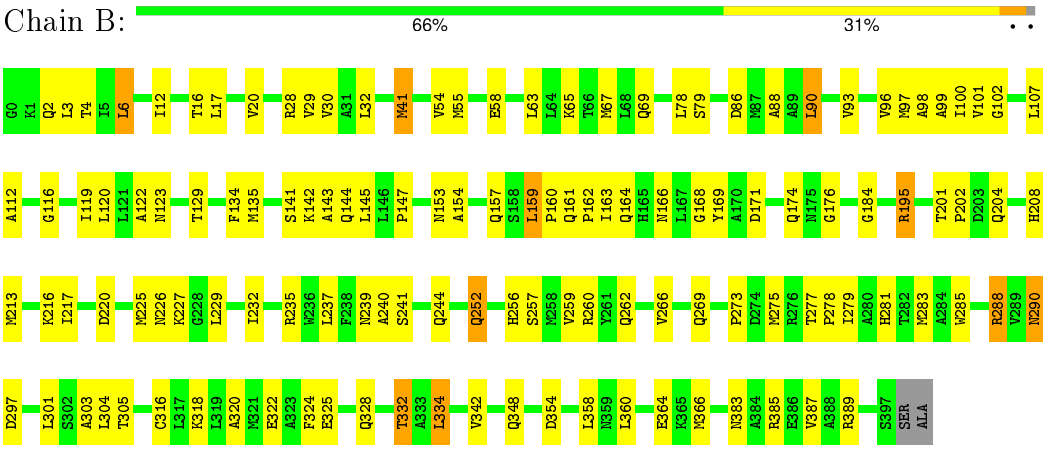
- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	182.16Å 59.19Å 87.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6446	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3067	0.59	0/4127
1	B	0.31	0/3055	0.57	0/4112
All	All	0.31	0/6122	0.58	0/8239

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3037	0	3059	142	0
1	B	3025	0	3049	116	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	48	0	26	2	0
3	B	48	0	26	1	0
4	A	148	0	0	8	0
4	B	130	0	0	6	0
All	All	6446	0	6160	247	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 20.

All (247) 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:366:MSE:HE1	1:B:387:VAL:HG21	1.39	1.02
1:A:296:LEU:HD11	1:B:266:VAL:HG21	1.45	0.97
1:A:337:ALA:HB2	1:A:362:VAL:HG21	1.53	0.90
1:B:12:ILE:O	1:B:16:THR:HG23	1.72	0.88
1:B:328:GLN:O	1:B:332:THR:HG23	1.74	0.88
1:A:225:MSE:HE1	1:A:334:LEU:HD22	1.56	0.87
1:A:67:MSE:HA	1:A:70:GLN:HE21	1.44	0.82
1:A:368:MSE:HE1	1:A:380:VAL:HA	1.62	0.81
1:B:201:THR:HG22	1:B:204:GLN:HG3	1.60	0.81
1:A:158:SER:O	1:A:259:VAL:HG11	1.82	0.79
1:A:225:MSE:HG2	1:A:316:CYS:HB3	1.64	0.78
1:B:97:MSE:HE3	1:B:98:ALA:N	1.99	0.78
1:A:241:SER:H	1:A:244:GLN:HE21	1.26	0.77
1:A:225:MSE:HE3	1:A:338:ASN:HB2	1.67	0.77
1:A:95:GLN:HB3	1:A:120:LEU:HD21	1.67	0.77
1:A:12:ILE:O	1:A:16:THR:HG22	1.85	0.76
1:B:217:ILE:H	1:B:217:ILE:HD12	1.50	0.75
1:B:241:SER:H	1:B:244:GLN:HE21	1.32	0.74
1:A:296:LEU:HD12	1:B:260:ARG:HH12	1.52	0.74
1:B:30:VAL:HG21	1:B:93:VAL:HG12	1.70	0.74
1:A:96:VAL:HG11	1:A:112:ALA:HB1	1.69	0.73
1:A:33:VAL:HG22	1:A:54:VAL:CG1	2.18	0.73
1:B:159:LEU:HD13	1:B:259:VAL:HG21	1.69	0.73
1:B:164:GLN:NE2	1:B:285:TRP:HE1	1.87	0.72
1:B:129:THR:HA	1:B:332:THR:HG22	1.72	0.71
1:A:33:VAL:HG22	1:A:54:VAL:HG13	1.72	0.71
1:A:337:ALA:CB	1:A:362:VAL:HG21	2.20	0.71
1:A:153:ASN:ND2	1:A:157:GLN:HE21	1.88	0.71
1:A:395:LEU:HD12	1:A:399:ALA:HB3	1.73	0.70
1:A:147:PRO:HG3	1:A:237:LEU:HD21	1.72	0.70
1:A:246:GLU:OE2	1:A:260:ARG:HD2	1.90	0.70
1:B:4:THR:CG2	1:B:96:VAL:HG22	2.21	0.70
1:B:208:HIS:HD2	1:B:213:MSE:HE2	1.58	0.69
1:A:23:ASN:ND2	1:A:289:VAL:HG22	2.09	0.68
1:A:68:LEU:HB3	1:A:73:SER:HB3	1.74	0.68
1:B:201:THR:HG22	1:B:204:GLN:CG	2.24	0.68
1:B:2:GLN:HE21	1:B:28:ARG:HE	1.42	0.67
1:A:153:ASN:HD21	1:A:157:GLN:HE21	1.41	0.67
1:A:120:LEU:N	1:A:120:LEU:HD22	2.08	0.67
1:A:225:MSE:CE	1:A:334:LEU:HD22	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MSE:O	1:A:278:PRO:HD2	1.96	0.65
1:A:107:LEU:HD21	1:A:374:VAL:HG21	1.77	0.65
1:B:275:MSE:O	1:B:278:PRO:HD2	1.98	0.64
1:A:225:MSE:HE3	1:A:338:ASN:CB	2.28	0.63
1:B:217:ILE:N	1:B:217:ILE:HD12	2.12	0.63
1:B:225:MSE:HE1	1:B:334:LEU:HD21	1.79	0.63
1:B:41:MSE:HG3	1:B:55:MSE:SE	2.48	0.63
1:A:241:SER:H	1:A:244:GLN:NE2	1.95	0.63
1:B:216:LYS:HD2	1:B:342:VAL:HG11	1.80	0.63
1:A:252:GLN:HE22	1:A:305:THR:H	1.45	0.63
1:A:303:ALA:HB1	1:B:303:ALA:HB1	1.81	0.62
1:A:296:LEU:HD12	1:B:260:ARG:NH1	2.14	0.62
1:B:20:VAL:HG12	1:B:283:MSE:HE1	1.82	0.62
1:B:67:MSE:HA	1:B:67:MSE:HE2	1.81	0.61
1:B:297:ASP:O	1:B:301:LEU:HD13	2.00	0.61
1:A:277:THR:HB	1:A:278:PRO:HD3	1.81	0.61
1:B:277:THR:HB	1:B:278:PRO:HD3	1.81	0.60
1:B:241:SER:H	1:B:244:GLN:NE2	1.99	0.60
1:B:97:MSE:HA	1:B:120:LEU:HB2	1.82	0.60
1:B:153:ASN:HD21	1:B:157:GLN:HE21	1.50	0.60
1:A:50:PRO:HD2	1:A:75:THR:HG21	1.82	0.60
1:A:315:PRO:HD2	4:A:2007:HOH:O	2.02	0.60
1:B:107:LEU:HD23	4:B:2016:HOH:O	2.01	0.60
1:B:161:GLN:HB3	1:B:162:PRO:HD3	1.84	0.60
1:B:201:THR:CG2	1:B:204:GLN:HG3	2.32	0.59
1:B:97:MSE:HE1	1:B:122:ALA:HB2	1.84	0.59
1:A:358:LEU:O	1:A:362:VAL:HG13	2.01	0.59
1:B:3:LEU:HD23	1:B:28:ARG:O	2.02	0.59
1:B:290:ASN:ND2	1:B:292:GLY:H	2.01	0.59
1:B:153:ASN:ND2	1:B:157:GLN:HE21	2.00	0.59
1:A:105:GLY:C	1:A:108:PRO:HD2	2.24	0.59
1:B:17:LEU:O	1:B:20:VAL:HG22	2.02	0.59
1:A:41:MSE:HG3	1:A:55:MSE:SE	2.52	0.58
1:B:288:ARG:HD3	4:B:2072:HOH:O	2.01	0.58
1:B:97:MSE:HE2	1:B:99:ALA:HB2	1.84	0.58
1:A:25:GLU:HG2	1:A:26:HIS:ND1	2.19	0.58
1:A:362:VAL:O	1:A:366:MSE:HG2	2.04	0.58
1:A:127:LEU:HD21	1:A:135:MSE:HE1	1.86	0.57
1:A:135:MSE:HE3	1:A:236:TRP:C	2.25	0.57
1:A:103:ALA:O	1:A:106:LEU:HB2	2.05	0.57
1:A:50:PRO:O	1:A:75:THR:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:HE3	1:A:169:TYR:CE1	2.40	0.56
1:B:232:ILE:CD1	1:B:324:PHE:HB2	2.35	0.56
1:A:348:GLN:HA	4:A:2026:HOH:O	2.05	0.56
1:A:368:MSE:CE	1:A:380:VAL:HA	2.33	0.56
1:A:65:LYS:HA	1:A:77:VAL:HG21	1.87	0.55
1:A:358:LEU:HD11	1:A:395:LEU:HD22	1.89	0.55
1:A:195:ARG:HD3	4:A:2105:HOH:O	2.06	0.55
1:B:147:PRO:HB3	1:B:237:LEU:HD21	1.89	0.55
1:B:86:ASP:O	1:B:90:LEU:HD13	2.07	0.55
1:A:226:ASN:HB3	4:A:2102:HOH:O	2.06	0.55
1:B:168:GLY:O	1:B:239:ASN:HB2	2.06	0.55
1:A:101:VAL:HG22	1:A:102:GLY:N	2.21	0.55
1:B:225:MSE:HE2	1:B:316:CYS:SG	2.47	0.55
1:A:252:GLN:NE2	1:A:305:THR:H	2.04	0.55
1:B:226:ASN:HB3	4:B:2088:HOH:O	2.07	0.54
1:B:216:LYS:HE2	1:B:220:ASP:OD1	2.07	0.54
1:B:252:GLN:NE2	1:B:252:GLN:H	2.05	0.54
1:A:67:MSE:HA	1:A:70:GLN:NE2	2.20	0.54
1:B:65:LYS:O	1:B:69:GLN:HG3	2.08	0.54
1:A:124:LYS:HE2	1:A:226:ASN:ND2	2.22	0.54
1:B:97:MSE:HE1	1:B:122:ALA:CB	2.38	0.54
1:A:367:ASP:O	1:A:369:ARG:HG2	2.08	0.53
1:A:120:LEU:H	1:A:120:LEU:HD22	1.70	0.53
1:B:2:GLN:NE2	1:B:28:ARG:HE	2.04	0.53
1:B:141:SER:O	1:B:142:LYS:HB2	2.08	0.53
1:B:6:LEU:HB3	1:B:100:ILE:HG13	1.91	0.53
1:B:360:LEU:O	1:B:364:GLU:HG3	2.09	0.53
1:A:281:HIS:HE1	4:A:2097:HOH:O	1.92	0.52
1:A:96:VAL:HG11	1:A:112:ALA:CB	2.39	0.52
1:A:105:GLY:CA	1:A:108:PRO:HD2	2.40	0.52
1:B:217:ILE:H	1:B:217:ILE:CD1	2.20	0.52
1:A:178:VAL:CG2	1:A:260:ARG:HB2	2.39	0.52
1:A:225:MSE:CE	1:A:338:ASN:HB2	2.39	0.52
1:A:135:MSE:O	1:A:138:VAL:HG22	2.11	0.52
1:A:134:PHE:O	1:A:138:VAL:HG13	2.10	0.51
1:B:256:HIS:HD2	1:B:269:GLN:OE1	1.93	0.51
1:A:164:GLN:NE2	1:A:285:TRP:HE1	2.09	0.51
1:B:201:THR:HG23	1:B:204:GLN:H	1.76	0.51
1:A:105:GLY:O	1:A:109:THR:HG22	2.10	0.51
1:B:135:MSE:HE2	1:B:168:GLY:HA3	1.92	0.51
1:A:5:ILE:CD1	1:A:17:LEU:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLY:HA2	1:B:143:ALA:HB2	1.92	0.51
1:A:256:HIS:HE1	4:A:2111:HOH:O	1.93	0.51
1:A:17:LEU:HG	1:A:48:PHE:CE1	2.45	0.51
1:A:225:MSE:HG2	1:A:316:CYS:CB	2.37	0.51
1:A:178:VAL:HG22	1:A:260:ARG:HB2	1.93	0.51
1:A:149:ASP:HA	3:A:2001:NDP:H5N	1.92	0.51
1:A:135:MSE:HE3	1:A:237:LEU:N	2.26	0.51
1:A:42:VAL:O	1:A:46:LEU:HG	2.10	0.51
1:A:158:SER:HB3	1:A:259:VAL:HG12	1.92	0.51
1:B:385:ARG:O	1:B:389:ARG:HG3	2.11	0.50
1:B:318:LYS:O	1:B:322:GLU:HG3	2.11	0.50
1:B:235:ARG:NH2	1:B:325:GLU:OE1	2.44	0.50
1:A:13:GLY:O	1:A:16:THR:HG23	2.11	0.50
1:A:184:GLY:HA3	1:A:227:LYS:HE3	1.93	0.50
1:B:256:HIS:HE1	4:B:2068:HOH:O	1.94	0.50
1:A:213:MSE:HB2	1:A:217:ILE:HD11	1.93	0.50
1:A:127:LEU:CD2	1:A:135:MSE:HE1	2.42	0.49
1:A:38:VAL:O	1:A:42:VAL:HG23	2.10	0.49
1:B:348:GLN:HA	4:B:2065:HOH:O	2.11	0.49
1:B:119:ILE:HB	1:B:145:LEU:HD23	1.94	0.49
1:A:298:PHE:HA	1:A:301:LEU:HD22	1.93	0.49
1:B:252:GLN:NE2	1:B:305:THR:H	2.10	0.49
1:A:213:MSE:HE3	1:A:217:ILE:CG1	2.41	0.49
1:A:147:PRO:CG	1:A:237:LEU:HD21	2.41	0.49
1:B:281:HIS:HE1	4:B:2010:HOH:O	1.95	0.49
1:A:106:LEU:O	1:A:109:THR:HG22	2.12	0.49
1:B:232:ILE:HD11	1:B:320:ALA:O	2.13	0.49
1:B:2:GLN:HE21	1:B:28:ARG:NE	2.08	0.49
1:B:275:MSE:C	1:B:278:PRO:HD2	2.33	0.49
1:B:107:LEU:HB2	1:B:108:PRO:HD3	1.95	0.48
1:B:171:ASP:OD1	1:B:174:GLN:HG2	2.12	0.48
1:A:366:MSE:HE1	1:A:368:MSE:HE2	1.95	0.48
1:B:4:THR:HG23	1:B:96:VAL:HG13	1.94	0.48
1:A:296:LEU:HD13	1:A:298:PHE:CE1	2.48	0.48
1:B:20:VAL:CG1	1:B:283:MSE:HE1	2.43	0.48
1:B:210:ASN:HB3	1:B:211:TRP:CE3	2.49	0.48
1:B:252:GLN:HE22	1:B:305:THR:H	1.61	0.48
1:B:184:GLY:HA3	1:B:227:LYS:HE3	1.96	0.47
1:B:135:MSE:CE	1:B:168:GLY:HA3	2.44	0.47
1:B:54:VAL:HG22	1:B:78:LEU:HB2	1.97	0.47
1:B:88:ALA:HB1	1:B:112:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:OG1	1:B:202:PRO:HD2	2.15	0.47
1:A:304:LEU:HB2	1:B:304:LEU:HB2	1.97	0.47
1:B:32:LEU:CB	1:B:41:MSE:HE1	2.45	0.47
1:B:166:ASN:HB3	1:B:169:TYR:CE1	2.50	0.47
1:B:90:LEU:HB3	1:B:93:VAL:HG13	1.96	0.47
1:A:366:MSE:CE	1:A:368:MSE:HE2	2.46	0.46
1:A:122:ALA:HB2	1:A:148:VAL:CG2	2.46	0.46
1:A:37:ASN:OD1	1:A:40:ARG:HB2	2.15	0.46
1:A:97:MSE:HA	1:A:120:LEU:HB2	1.96	0.46
1:A:181:LEU:HD11	1:A:260:ARG:HD2	1.97	0.46
1:A:73:SER:OG	1:A:75:THR:HG23	2.15	0.46
1:B:29:VAL:HG11	1:B:32:LEU:HD21	1.97	0.46
1:A:29:VAL:HG11	1:A:32:LEU:HD21	1.96	0.46
1:B:290:ASN:HD22	1:B:291:SER:N	2.13	0.46
1:B:235:ARG:HD2	1:B:240:ALA:O	2.16	0.46
1:A:133:LEU:H	1:A:328:GLN:HE22	1.64	0.46
1:B:101:VAL:HG22	1:B:102:GLY:N	2.30	0.46
1:B:164:GLN:HE22	1:B:285:TRP:HE1	1.64	0.45
1:A:110:LEU:O	1:A:114:ARG:HG2	2.15	0.45
1:A:139:LYS:HE3	1:A:169:TYR:HE1	1.81	0.45
1:A:212:SER:HA	4:A:2128:HOH:O	2.16	0.45
1:A:135:MSE:HE2	1:A:236:TRP:HB3	1.99	0.45
1:B:90:LEU:O	1:B:93:VAL:HG22	2.16	0.45
1:A:107:LEU:CD2	1:A:374:VAL:HG21	2.46	0.45
1:B:290:ASN:HD22	1:B:291:SER:H	1.64	0.45
1:A:135:MSE:HE3	1:A:237:LEU:HA	1.98	0.45
1:A:115:ALA:HB3	1:A:117:LYS:HD3	1.99	0.45
1:A:141:SER:O	1:A:142:LYS:HB2	2.16	0.45
1:A:275:MSE:C	1:A:278:PRO:HD2	2.37	0.44
1:A:9:THR:HG22	1:A:40:ARG:HB3	2.00	0.44
1:A:258:MSE:HG2	1:A:268:ALA:HB2	2.00	0.44
1:B:16:THR:HG22	1:B:279:ILE:HD13	2.00	0.44
1:B:211:TRP:CH2	1:B:273:PRO:HG3	2.52	0.44
1:B:195:ARG:H	1:B:195:ARG:CD	2.30	0.44
1:A:21:ARG:O	1:A:24:PRO:HD3	2.18	0.44
1:A:296:LEU:HD11	1:B:266:VAL:CG2	2.32	0.44
1:B:220:ASP:HB3	1:B:226:ASN:HB2	2.00	0.44
1:B:110:LEU:HG	1:B:134:PHE:CE2	2.53	0.44
1:A:344:ALA:HA	1:A:349:GLN:HE21	1.83	0.43
1:A:258:MSE:HG2	1:A:268:ALA:CB	2.48	0.43
1:A:161:GLN:HB3	1:A:162:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MSE:HA	1:A:70:GLN:HG2	2.01	0.43
1:B:157:GLN:HG2	1:B:281:HIS:CE1	2.54	0.43
1:A:318:LYS:O	1:A:322:GLU:HG3	2.18	0.43
1:A:225:MSE:HE3	1:A:338:ASN:CG	2.38	0.43
1:A:96:VAL:C	1:A:120:LEU:HD23	2.39	0.43
1:A:214:GLY:H	1:A:217:ILE:HD11	1.84	0.43
1:A:101:VAL:CG2	1:A:102:GLY:N	2.81	0.43
1:B:195:ARG:N	1:B:195:ARG:HD3	2.34	0.43
1:A:83:ALA:O	1:A:87:MSE:HG2	2.19	0.43
1:A:232:ILE:HG23	1:A:324:PHE:HD1	1.83	0.43
1:B:154:ALA:HB1	1:B:269:GLN:HB3	2.01	0.42
1:A:141:SER:HB3	4:A:2045:HOH:O	2.18	0.42
1:A:366:MSE:HE1	1:A:383:ASN:HD22	1.84	0.42
1:A:124:LYS:HE2	1:A:226:ASN:HD21	1.84	0.42
1:B:210:ASN:HB3	1:B:211:TRP:CZ3	2.53	0.42
1:A:120:LEU:N	1:A:120:LEU:CD2	2.79	0.42
1:A:131:GLY:HA3	1:A:236:TRP:CD1	2.54	0.42
1:A:213:MSE:HE3	1:A:217:ILE:HB	2.00	0.42
1:A:290:ASN:HB2	1:B:262:GLN:HE21	1.85	0.42
1:A:61:ALA:CB	1:A:79:SER:HB3	2.50	0.42
1:A:260:ARG:NH2	1:B:296:LEU:O	2.28	0.42
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.85	0.42
1:A:252:GLN:H	1:A:252:GLN:NE2	2.18	0.41
1:A:36:LYS:HG2	1:A:57:ASP:HB2	2.02	0.41
1:A:122:ALA:HB2	1:A:148:VAL:HG21	2.03	0.41
1:B:275:MSE:HE2	3:B:2002:NDP:H42N	2.02	0.41
1:B:32:LEU:HB2	1:B:41:MSE:HE1	2.03	0.41
1:A:208:HIS:HA	1:A:209:PRO:HD3	1.89	0.41
1:A:181:LEU:HD13	1:A:260:ARG:HG3	2.02	0.41
1:B:55:MSE:O	1:B:79:SER:HA	2.21	0.41
1:A:288:ARG:HB2	1:B:176:GLY:HA3	2.02	0.41
1:A:370:GLU:HA	1:A:371:PRO:HD2	1.87	0.41
1:B:63:LEU:O	1:B:67:MSE:HG2	2.20	0.41
1:A:32:LEU:O	1:A:41:MSE:HE1	2.20	0.41
1:B:171:ASP:CG	1:B:174:GLN:HG2	2.42	0.41
1:A:288:ARG:CB	1:B:176:GLY:HA3	2.51	0.41
1:A:295:PRO:HB3	1:B:260:ARG:HD3	2.02	0.40
1:B:354:ASP:O	1:B:358:LEU:HB2	2.21	0.40
1:B:195:ARG:H	1:B:195:ARG:NE	2.19	0.40
1:B:160:PRO:CG	1:B:163:ILE:HD12	2.51	0.40
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:O	3:A:2001:NDP:O4D	2.38	0.40
1:A:213:MSE:HE3	1:A:217:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	398/400 (100%)	382 (96%)	13 (3%)	3 (1%)	24 22
1	B	396/400 (99%)	387 (98%)	8 (2%)	1 (0%)	46 50
All	All	794/800 (99%)	769 (97%)	21 (3%)	4 (0%)	34 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	SER
1	B	257	SER
1	A	397	SER
1	A	370	GLU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/310 (106%)	298 (91%)	30 (9%)	12	11
1	B	327/310 (106%)	310 (95%)	17 (5%)	29	33
All	All	655/620 (106%)	608 (93%)	47 (7%)	18	18

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	16	THR
1	A	17	LEU
1	A	41	MSE
1	A	54	VAL
1	A	75	THR
1	A	97	MSE
1	A	114	ARG
1	A	135	MSE
1	A	144	GLN
1	A	146	LEU
1	A	148	VAL
1	A	159	LEU
1	A	166	ASN
1	A	191	GLU
1	A	194	LEU
1	A	225	MSE
1	A	229	LEU
1	A	252	GLN
1	A	257	SER
1	A	267	LEU
1	A	288	ARG
1	A	289	VAL
1	A	296	LEU
1	A	301	LEU
1	A	317	LEU
1	A	334	LEU
1	A	372	GLN
1	A	377	VAL
1	A	378	LEU
1	B	6	LEU
1	B	41	MSE

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Mol	Chain	Res	Type
1	B	58	GLU
1	B	90	LEU
1	B	110	LEU
1	B	123	ASN
1	B	144	GLN
1	B	159	LEU
1	B	195	ARG
1	B	211	TRP
1	B	229	LEU
1	B	252	GLN
1	B	288	ARG
1	B	290	ASN
1	B	332	THR
1	B	334	LEU
1	B	383	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	70	GLN
1	A	95	GLN
1	A	123	ASN
1	A	153	ASN
1	A	164	GLN
1	A	166	ASN
1	A	175	ASN
1	A	226	ASN
1	A	239	ASN
1	A	244	GLN
1	A	252	GLN
1	A	256	HIS
1	A	262	GLN
1	A	281	HIS
1	A	328	GLN
1	A	349	GLN
1	A	383	ASN
1	B	2	GLN
1	B	81	GLN
1	B	82	GLN
1	B	123	ASN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	166	ASN
1	B	175	ASN
1	B	244	GLN
1	B	252	GLN
1	B	256	HIS
1	B	262	GLN
1	B	281	HIS
1	B	290	ASN
1	B	372	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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1001	-	4,4,4	0.18	0	6,6,6	0.09	0
3	NDP	A	2001	-	42,52,52	1.62	8 (19%)	55,80,80	1.47	7 (12%)
2	SO4	B	1002	-	4,4,4	0.17	0	6,6,6	0.06	0
3	NDP	B	2002	-	42,52,52	1.62	7 (16%)	55,80,80	1.49	7 (12%)

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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	NDP	A	2001	-	-	0/30/77/77	0/5/5/5
2	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
3	NDP	B	2002	-	-	0/30/77/77	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	NDP	C4N-C5N	-6.08	1.36	1.49
3	B	2002	NDP	C4N-C5N	-5.99	1.36	1.49
3	A	2001	NDP	PA-O2A	-2.37	1.44	1.54
3	B	2002	NDP	PA-O2A	-2.32	1.45	1.54
3	A	2001	NDP	P2B-O2X	-2.22	1.46	1.54
3	B	2002	NDP	P2B-O3X	-2.20	1.46	1.54
3	B	2002	NDP	P2B-O2X	-2.17	1.46	1.54
3	A	2001	NDP	P2B-O3X	-2.15	1.47	1.54
3	A	2001	NDP	O4B-C1B	2.00	1.43	1.41
3	A	2001	NDP	C4A-N3A	2.03	1.38	1.35
3	B	2002	NDP	O4B-C1B	2.17	1.43	1.41
3	A	2001	NDP	C6N-C5N	2.76	1.38	1.33
3	B	2002	NDP	C6N-C5N	2.91	1.38	1.33
3	A	2001	NDP	C2N-C3N	4.26	1.45	1.34
3	B	2002	NDP	C2N-C3N	4.36	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	NDP	N3A-C2A-N1A	-4.97	125.09	128.89
3	A	2001	NDP	N3A-C2A-N1A	-4.82	125.20	128.89
3	A	2001	NDP	C3N-C2N-N1N	-4.28	117.01	123.14
3	B	2002	NDP	C3N-C2N-N1N	-4.13	117.22	123.14
3	B	2002	NDP	O7N-C7N-N7N	-2.51	116.53	122.76
3	A	2001	NDP	O7N-C7N-N7N	-2.39	116.82	122.76
3	A	2001	NDP	C4N-C5N-C6N	-2.19	118.97	122.58
3	B	2002	NDP	C4N-C5N-C6N	-2.17	119.00	122.58
3	A	2001	NDP	PN-O3-PA	2.39	139.44	132.73
3	B	2002	NDP	PN-O3-PA	2.81	140.63	132.73
3	A	2001	NDP	O3-PN-O5D	2.86	110.53	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2002	NDP	O3-PN-O5D	3.03	110.97	102.94
3	A	2001	NDP	C5N-C4N-C3N	3.95	123.41	112.52
3	B	2002	NDP	C5N-C4N-C3N	3.98	123.48	112.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NDP	2	0
3	B	2002	NDP	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.