



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 PM UTC

PDB ID : 1KC7 / pdb_00001kc7
Title : Pyruvate Phosphate Dikinase with Bound Mg-phosphonopyruvate
Authors : Chen, C.C.; Howard, A.; Herzberg, O.
Deposited on : 2001-11-07
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

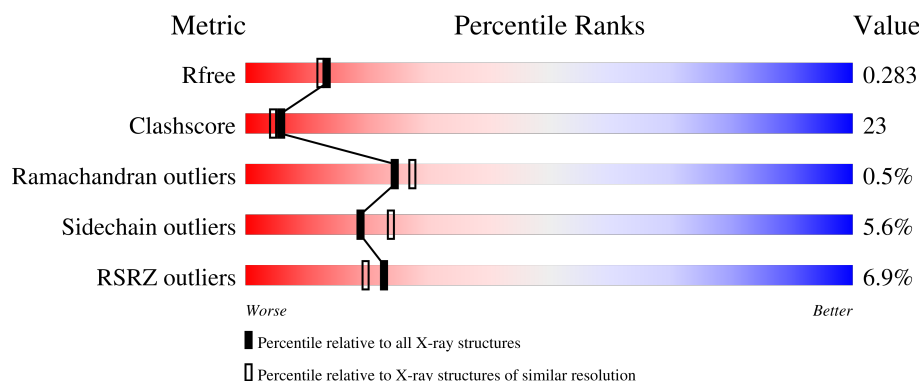
1 Overall quality at a glance

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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	873	

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
4	PPR	A	1000	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6783 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.

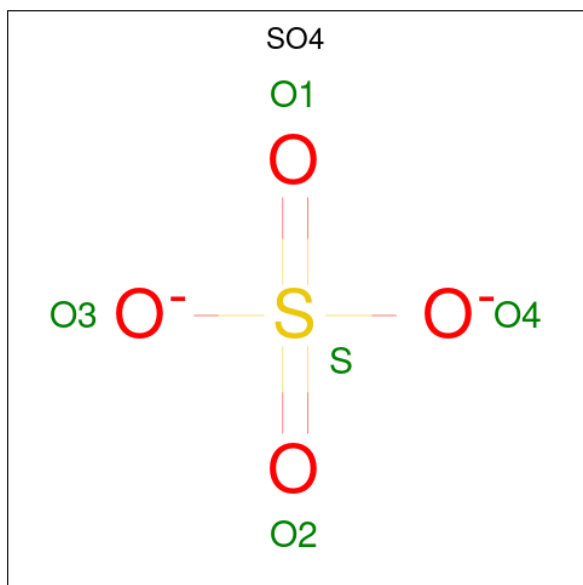
- Molecule 1 is a protein called pyruvate phosphate dikinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	872	Total	C	N	O	S	41	0	0
			6752	4250	1143	1308	51			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



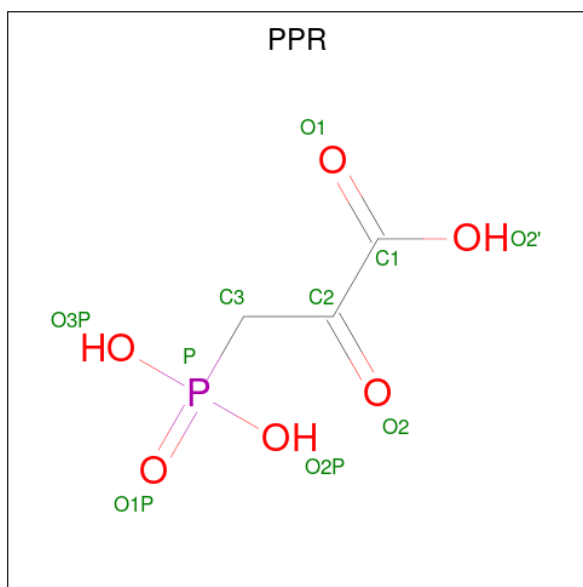
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is PHOSPHONOPYRUVATE (CCD ID: PPR) (formula: $C_3H_5O_6P$).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.21Å 58.42Å 102.55Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 25.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.00-2.20) 97.0 (25.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 1.73Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.198 , 0.269 0.241 , 0.283	Depositor DCC
R_{free} test set	4605 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.99	12/6876 (0.2%)	1.31	79/9269 (0.9%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	MET	SD-CE	-9.32	1.56	1.79
1	A	812	VAL	CA-C	9.11	1.64	1.52
1	A	749	ALA	CA-CB	-8.02	1.40	1.53
1	A	310	MET	SD-CE	7.33	1.97	1.79
1	A	744	ILE	CA-C	-5.91	1.46	1.52
1	A	813	GLU	N-CA	5.81	1.53	1.46
1	A	322	MET	SD-CE	-5.47	1.65	1.79
1	A	830	ILE	CA-CB	5.32	1.62	1.54
1	A	554	ALA	CA-CB	5.26	1.61	1.53
1	A	812	VAL	CA-CB	5.22	1.60	1.54
1	A	677	ALA	CA-CB	5.14	1.61	1.53
1	A	769	ASP	CA-C	-5.10	1.46	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ARG	CA-C-N	-15.43	105.25	120.52
1	A	612	ARG	C-N-CA	-15.43	105.25	120.52
1	A	519	GLY	N-CA-C	-12.31	95.75	112.25
1	A	488	HIS	N-CA-C	9.69	122.53	108.86
1	A	621	PRO	N-CA-C	9.12	121.83	110.70
1	A	768	ASN	N-CA-C	-9.12	101.29	111.14
1	A	521	PHE	N-CA-C	-8.09	100.81	111.24
1	A	229	ILE	CB-CA-C	-7.94	101.72	110.85
1	A	399	SER	CA-C-N	7.91	127.83	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	SER	C-N-CA	7.91	127.83	119.85
1	A	339	GLY	N-CA-C	7.90	122.29	111.54
1	A	429	LEU	N-CA-C	-7.78	102.75	111.07
1	A	43	THR	N-CA-C	7.68	120.50	110.43
1	A	20	GLY	N-CA-C	-7.42	103.36	112.33
1	A	143	VAL	N-CA-C	7.25	117.34	110.30
1	A	746	ILE	N-CA-C	-7.10	99.16	107.61
1	A	285	VAL	N-CA-C	-7.07	103.88	110.53
1	A	378	HIS	CA-C-N	-7.04	112.51	119.76
1	A	378	HIS	C-N-CA	-7.04	112.51	119.76
1	A	286	ARG	N-CA-C	-6.99	97.85	108.96
1	A	163	LYS	N-CA-C	-6.80	103.99	113.37
1	A	423	ARG	N-CA-C	-6.70	99.61	110.20
1	A	780	ASP	N-CA-C	6.68	119.40	111.71
1	A	248	GLY	N-CA-C	6.64	119.09	110.45
1	A	270	GLY	N-CA-C	6.55	119.28	110.43
1	A	557	ILE	N-CA-C	6.49	117.37	107.77
1	A	659	ASN	CA-C-N	6.48	126.99	119.47
1	A	659	ASN	C-N-CA	6.48	126.99	119.47
1	A	535	LYS	N-CA-C	-6.39	101.06	110.52
1	A	300	ASP	N-CA-C	6.31	118.16	111.28
1	A	145	MET	N-CA-C	-6.30	97.38	110.80
1	A	542	THR	CA-C-N	6.17	125.66	119.24
1	A	542	THR	C-N-CA	6.17	125.66	119.24
1	A	607	LYS	N-CA-C	-6.12	104.24	111.03
1	A	832	GLY	N-CA-C	-6.00	102.22	112.30
1	A	595	ILE	CA-C-N	-5.96	112.43	119.05
1	A	595	ILE	C-N-CA	-5.96	112.43	119.05
1	A	616	VAL	CB-CA-C	-5.89	103.83	110.96
1	A	229	ILE	N-CA-C	-5.88	101.03	107.73
1	A	846	LYS	N-CA-C	5.79	118.37	111.71
1	A	599	LYS	N-CA-C	-5.79	105.06	111.71
1	A	691	VAL	N-CA-C	-5.76	103.85	111.05
1	A	42	VAL	N-CA-C	-5.76	99.42	108.23
1	A	788	SER	N-CA-C	-5.73	105.17	111.82
1	A	177	LYS	N-CA-C	-5.73	105.04	111.28
1	A	7	LYS	N-CA-C	-5.72	102.83	110.55
1	A	349	ILE	N-CA-C	5.70	115.90	110.42
1	A	409	PHE	N-CA-C	5.65	120.16	112.88
1	A	144	VAL	N-CA-C	5.64	116.42	110.72
1	A	65	ILE	N-CA-C	-5.63	105.13	110.42
1	A	461	ARG	N-CA-C	-5.61	104.54	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	VAL	N-CA-C	5.58	117.35	108.87
1	A	808	VAL	CB-CA-C	-5.55	104.65	112.14
1	A	524	ILE	N-CA-C	-5.52	105.15	110.72
1	A	514	GLU	N-CA-C	5.51	118.52	109.76
1	A	16	ARG	N-CA-C	5.48	117.97	111.33
1	A	104	ASP	N-CA-C	5.48	118.42	109.59
1	A	690	GLU	N-CA-C	5.48	116.93	111.07
1	A	669	LEU	N-CA-C	-5.47	105.34	112.23
1	A	243	VAL	N-CA-C	-5.45	100.33	108.46
1	A	442	ALA	N-CA-C	5.41	118.49	110.48
1	A	767	THR	N-CA-C	5.37	119.67	113.18
1	A	743	MET	N-CA-C	-5.30	101.89	110.32
1	A	443	GLU	N-CA-C	-5.29	105.59	111.36
1	A	20	GLY	CA-C-O	-5.27	118.36	122.52
1	A	36	ILE	CB-CA-C	-5.26	104.73	110.78
1	A	76	ASN	N-CA-C	5.23	119.37	112.89
1	A	468	VAL	N-CA-C	-5.23	100.12	107.75
1	A	48	THR	N-CA-C	-5.16	105.55	111.07
1	A	87	LEU	N-CA-C	-5.16	100.90	109.46
1	A	268	ILE	N-CA-C	5.15	116.32	109.37
1	A	620	ASP	N-CA-C	5.12	121.11	109.81
1	A	714	LEU	N-CA-C	-5.11	105.79	111.36
1	A	821	GLN	N-CA-C	-5.09	105.82	112.23
1	A	303	LYS	N-CA-C	-5.05	105.46	110.97
1	A	315	HIS	N-CA-C	5.05	116.60	111.14
1	A	487	GLY	N-CA-C	5.04	119.22	112.77
1	A	367	ARG	N-CA-C	5.03	117.88	111.69
1	A	763	PHE	CB-CA-C	-5.02	100.53	109.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6752	0	6668	307	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	20	0	0	0	0
4	A	10	0	2	1	0
All	All	6783	0	6670	307	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 23.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ALA:HA	1:A:322:MET:HE1	1.19	1.16
1:A:172:THR:HG22	1:A:174:ASP:H	1.07	1.14
1:A:579:ILE:HD11	1:A:623:LEU:HD22	1.26	1.13
1:A:396:LEU:HB3	1:A:452:MET:CE	1.84	1.07
1:A:396:LEU:HB3	1:A:452:MET:HE3	1.39	1.04
1:A:65:ILE:HG21	1:A:205:MET:HE1	1.45	0.99
1:A:557:ILE:HD13	1:A:609:LEU:HD21	1.50	0.94
1:A:322:MET:HE2	1:A:333:PHE:HE2	1.31	0.93
1:A:172:THR:HG22	1:A:174:ASP:N	1.83	0.92
1:A:34:MET:HE3	1:A:308:LEU:HD22	1.48	0.92
1:A:144:VAL:HG12	1:A:145:MET:HE2	1.51	0.92
1:A:106:ILE:HD11	1:A:143:VAL:HG11	1.51	0.90
1:A:309:ALA:CA	1:A:322:MET:HE1	2.02	0.89
1:A:312:LEU:HD12	1:A:322:MET:CE	2.05	0.87
1:A:518:SER:O	1:A:521:PHE:HB3	1.77	0.85
1:A:309:ALA:HA	1:A:322:MET:CE	2.07	0.84
1:A:576:ARG:HD3	1:A:626:PHE:O	1.81	0.81
1:A:579:ILE:CD1	1:A:623:LEU:HD22	2.08	0.80
1:A:529:ASP:CG	1:A:863:ARG:HH21	1.90	0.79
1:A:156:ILE:HG13	1:A:179:LEU:HD21	1.65	0.79
1:A:556:GLY:C	1:A:557:ILE:HD12	2.09	0.78
1:A:360:THR:OG1	1:A:363:GLU:HG3	1.84	0.77
1:A:743:MET:C	1:A:744:ILE:HD12	2.09	0.77
1:A:165:VAL:HG13	1:A:170:ASP:HB2	1.68	0.76
1:A:312:LEU:HD12	1:A:322:MET:HE3	1.68	0.76
1:A:322:MET:HE2	1:A:333:PHE:CE2	2.19	0.75
1:A:468:VAL:HG11	1:A:505:ILE:HD11	1.68	0.75
1:A:133:TYR:O	1:A:137:ILE:HG12	1.86	0.75
1:A:317:ARG:HH22	1:A:363:GLU:CD	1.94	0.75
1:A:678:LYS:HG2	1:A:720:VAL:CG1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HG2	1:A:79:LYS:HA	1.69	0.74
1:A:223:TYR:HD2	1:A:436:ILE:HD11	1.52	0.73
1:A:167:PHE:HB3	1:A:169:THR:HG23	1.72	0.70
1:A:189:GLU:HG3	1:A:189:GLU:O	1.90	0.70
1:A:396:LEU:HD12	1:A:451:GLY:HA2	1.72	0.70
1:A:505:ILE:N	1:A:505:ILE:HD12	2.06	0.70
1:A:4:TRP:H	1:A:64:GLN:HE22	1.40	0.70
1:A:144:VAL:CG1	1:A:145:MET:HE2	2.22	0.70
1:A:580:LEU:HD23	1:A:651:LYS:HG2	1.75	0.68
1:A:580:LEU:HB2	1:A:641:MET:HE1	1.74	0.68
1:A:425:ILE:HG21	1:A:496:ILE:HD11	1.75	0.68
1:A:381:PHE:CE1	1:A:510:ILE:HB	2.29	0.68
1:A:223:TYR:HD2	1:A:436:ILE:CD1	2.06	0.68
1:A:312:LEU:HD12	1:A:322:MET:HE2	1.73	0.68
1:A:529:ASP:OD2	1:A:863:ARG:NH2	2.28	0.67
1:A:223:TYR:CD2	1:A:436:ILE:HD11	2.29	0.67
1:A:678:LYS:HB3	1:A:724:VAL:HG21	1.77	0.67
1:A:705:ILE:HD12	1:A:705:ILE:N	2.11	0.66
1:A:32:LEU:HD22	1:A:311:LYS:NZ	2.09	0.66
1:A:268:ILE:HD11	1:A:305:PHE:HE2	1.60	0.66
1:A:754:ASP:O	1:A:822:THR:HG21	1.96	0.66
1:A:628:PRO:HG2	1:A:634:GLN:HG2	1.76	0.65
1:A:151:HIS:O	1:A:155:ILE:HG12	1.97	0.65
1:A:396:LEU:HB3	1:A:452:MET:HE1	1.76	0.65
1:A:4:TRP:H	1:A:64:GLN:NE2	1.94	0.65
1:A:557:ILE:HD13	1:A:609:LEU:CD2	2.25	0.64
1:A:165:VAL:CG1	1:A:170:ASP:HB2	2.28	0.64
1:A:599:LYS:HE2	1:A:686:GLU:HB3	1.79	0.64
1:A:172:THR:HB	1:A:175:ASP:OD2	1.98	0.64
1:A:644:THR:HG23	1:A:647:GLU:OE1	1.97	0.64
1:A:80:PHE:HA	1:A:87:LEU:HB3	1.79	0.64
1:A:66:PHE:CE1	1:A:205:MET:HE3	2.33	0.64
1:A:96:ARG:HD2	1:A:233:TRP:CZ3	2.34	0.63
1:A:482:THR:HG22	1:A:491:ALA:HA	1.80	0.63
1:A:627:VAL:CG2	1:A:652:VAL:HG22	2.28	0.63
1:A:317:ARG:NH2	1:A:363:GLU:OE2	2.31	0.63
1:A:221:ILE:HD13	1:A:224:ARG:NH2	2.13	0.63
1:A:519:GLY:O	1:A:520:SER:HB2	1.99	0.63
1:A:343:ALA:HB3	1:A:344:PRO:HD3	1.81	0.63
1:A:162:GLU:C	1:A:164:GLY:H	2.05	0.62
1:A:572:ILE:HG23	1:A:573:MET:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ALA:HB1	1:A:786:LEU:HD22	1.81	0.62
1:A:62:GLN:HE21	1:A:205:MET:HG3	1.64	0.62
1:A:434:GLU:OE1	1:A:434:GLU:N	2.21	0.62
1:A:65:ILE:CG2	1:A:205:MET:HE1	2.26	0.61
1:A:96:ARG:HD2	1:A:233:TRP:CE3	2.34	0.61
1:A:268:ILE:HD11	1:A:305:PHE:CE2	2.35	0.61
1:A:354:VAL:HG11	1:A:527:TRP:CH2	2.35	0.61
1:A:578:MET:HE3	1:A:591:LEU:HD21	1.81	0.61
1:A:830:ILE:HG22	1:A:852:VAL:HA	1.81	0.61
1:A:627:VAL:HG21	1:A:652:VAL:HG22	1.83	0.60
1:A:436:ILE:HG23	1:A:437:GLU:N	2.15	0.60
1:A:226:MET:HE3	1:A:440:HIS:HD2	1.66	0.60
1:A:520:SER:HA	1:A:523:ARG:HB2	1.83	0.59
1:A:744:ILE:HD12	1:A:744:ILE:N	2.17	0.59
1:A:268:ILE:HD12	1:A:306:MET:SD	2.42	0.59
1:A:707:LEU:HD23	1:A:746:ILE:HD11	1.85	0.59
1:A:495:TYR:CD2	1:A:509:ASP:HB2	2.37	0.58
1:A:689:ILE:O	1:A:693:GLU:HG3	2.02	0.58
1:A:226:MET:HE3	1:A:440:HIS:CD2	2.38	0.58
1:A:447:THR:OG1	1:A:469:SER:HB2	2.04	0.58
1:A:817:LYS:O	1:A:821:GLN:HG3	2.03	0.58
1:A:131:ASP:O	1:A:134:ARG:HG3	2.03	0.58
1:A:156:ILE:HG13	1:A:179:LEU:CD2	2.34	0.58
1:A:209:LYS:O	1:A:213:ARG:HB2	2.03	0.58
1:A:406:LYS:HG2	1:A:495:TYR:CE1	2.38	0.58
1:A:38:GLN:O	1:A:241:THR:HG22	2.04	0.57
1:A:188:LYS:C	1:A:190:ALA:H	2.11	0.57
1:A:396:LEU:HD13	1:A:452:MET:HE3	1.85	0.57
1:A:488:HIS:CG	1:A:489:THR:H	2.22	0.57
1:A:742:THR:HG23	1:A:744:ILE:HD11	1.87	0.57
1:A:632:GLU:O	1:A:635:ALA:HB3	2.05	0.57
1:A:644:THR:OG1	1:A:647:GLU:HG3	2.05	0.57
1:A:519:GLY:C	1:A:521:PHE:H	2.12	0.56
1:A:79:LYS:CB	1:A:82:ASP:HB2	2.35	0.56
1:A:505:ILE:N	1:A:505:ILE:CD1	2.69	0.56
1:A:293:GLN:O	1:A:296:ASN:HB2	2.05	0.56
1:A:354:VAL:HG21	1:A:527:TRP:CZ3	2.41	0.56
1:A:390:GLU:O	1:A:392:ILE:HG23	2.06	0.56
1:A:454:SER:O	1:A:458:VAL:HG13	2.05	0.56
1:A:514:GLU:HG2	1:A:515:ALA:O	2.05	0.56
1:A:130:TYR:CZ	1:A:177:LYS:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:NH1	1:A:266:LYS:HG3	2.21	0.56
1:A:185:ALA:O	1:A:189:GLU:HB3	2.06	0.56
1:A:520:SER:O	1:A:524:ILE:HG12	2.06	0.56
1:A:630:THR:HG22	1:A:632:GLU:H	1.71	0.56
1:A:379:PRO:HB2	1:A:512:THR:OG1	2.05	0.55
1:A:78:LYS:NZ	1:A:85:ASP:OD1	2.39	0.55
1:A:128:PHE:CZ	1:A:247:LYS:HG3	2.42	0.55
1:A:584:VAL:O	1:A:588:GLU:HG3	2.06	0.55
1:A:617:ARG:NH2	4:A:1000:PPR:O3P	2.40	0.55
1:A:112:ASN:O	1:A:116:VAL:HG12	2.06	0.55
1:A:704:MET:SD	1:A:743:MET:HG2	2.47	0.55
1:A:573:MET:HE1	1:A:576:ARG:HH21	1.72	0.55
1:A:325:THR:OG1	1:A:334:LEU:HD11	2.07	0.54
1:A:580:LEU:HD12	1:A:641:MET:SD	2.48	0.54
1:A:423:ARG:HH22	1:A:509:ASP:CG	2.15	0.54
1:A:707:LEU:HA	1:A:746:ILE:CD1	2.38	0.54
1:A:565:MET:HB3	1:A:598:GLN:HG2	1.90	0.54
1:A:628:PRO:HB3	1:A:633:GLU:HG2	1.90	0.53
1:A:504:LYS:C	1:A:505:ILE:HD12	2.33	0.53
1:A:262:SER:HB3	1:A:400:PRO:HD3	1.88	0.53
1:A:704:MET:SD	1:A:764:SER:HB3	2.49	0.53
1:A:572:ILE:O	1:A:576:ARG:HG3	2.09	0.53
1:A:268:ILE:CD1	1:A:305:PHE:HE2	2.22	0.52
1:A:109:LEU:HA	1:A:136:PHE:CE1	2.44	0.52
1:A:289:GLN:HE21	1:A:293:GLN:CD	2.17	0.52
1:A:678:LYS:HG2	1:A:720:VAL:HG13	1.90	0.52
1:A:689:ILE:HD12	1:A:734:SER:OG	2.10	0.52
1:A:113:ASP:OD1	1:A:184:LYS:NZ	2.42	0.52
1:A:681:THR:OG1	1:A:721:VAL:HG13	2.10	0.52
1:A:414:ALA:HB1	1:A:424:VAL:HG11	1.91	0.51
1:A:34:MET:SD	1:A:312:LEU:HD21	2.51	0.51
1:A:579:ILE:HD12	1:A:623:LEU:HD13	1.92	0.51
1:A:573:MET:CE	1:A:576:ARG:HH21	2.24	0.51
1:A:79:LYS:HB3	1:A:82:ASP:HB2	1.93	0.51
1:A:274:ILE:HD11	1:A:297:ASP:OD2	2.11	0.51
1:A:635:ALA:HA	1:A:645:LEU:HD13	1.93	0.51
1:A:757:ALA:HB3	1:A:822:THR:OG1	2.10	0.50
1:A:396:LEU:CB	1:A:452:MET:HE3	2.28	0.50
1:A:7:LYS:HB2	1:A:10:GLU:HG3	1.93	0.50
1:A:189:GLU:O	1:A:189:GLU:CG	2.58	0.50
1:A:317:ARG:O	1:A:367:ARG:NH1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ALA:N	1:A:494:ASP:OD2	2.37	0.50
1:A:392:ILE:HG13	1:A:485:LEU:HD23	1.94	0.50
1:A:856:PRO:O	1:A:859:VAL:HG23	2.12	0.50
1:A:222:VAL:HG12	1:A:223:TYR:N	2.26	0.50
1:A:373:LEU:HD11	1:A:864:LEU:HD22	1.93	0.50
1:A:708:VAL:O	1:A:749:ALA:HB2	2.13	0.49
1:A:133:TYR:CE1	1:A:137:ILE:HD11	2.48	0.49
1:A:742:THR:HG23	1:A:744:ILE:CD1	2.42	0.49
1:A:787:ASP:OD2	1:A:791:LYS:HE3	2.12	0.49
1:A:381:PHE:HE1	1:A:510:ILE:HB	1.77	0.49
1:A:830:ILE:HD13	1:A:831:CYS:N	2.28	0.49
1:A:744:ILE:HD11	1:A:763:PHE:CD1	2.48	0.49
1:A:672:THR:O	1:A:674:PRO:HD3	2.13	0.49
1:A:677:ALA:O	1:A:678:LYS:C	2.55	0.48
1:A:32:LEU:HD22	1:A:311:LYS:HZ3	1.76	0.48
1:A:711:LYS:HD3	1:A:755:ALA:O	2.14	0.48
1:A:763:PHE:CD2	1:A:826:LEU:HD21	2.48	0.48
1:A:66:PHE:HE1	1:A:205:MET:HE3	1.77	0.48
1:A:276:ALA:HB2	1:A:286:ARG:HH22	1.78	0.48
1:A:722:VAL:HG23	1:A:740:ILE:HD12	1.95	0.48
1:A:714:LEU:HD21	1:A:760:ALA:HB2	1.96	0.48
1:A:223:TYR:HB2	1:A:436:ILE:CD1	2.43	0.48
1:A:375:GLN:HA	1:A:378:HIS:CE1	2.48	0.48
1:A:258:THR:O	1:A:259:ARG:HG2	2.13	0.48
1:A:415:LYS:O	1:A:419:GLU:HG2	2.13	0.48
1:A:223:TYR:CD2	1:A:436:ILE:CD1	2.92	0.48
1:A:518:SER:C	1:A:519:GLY:O	2.50	0.48
1:A:59:GLN:CD	1:A:59:GLN:H	2.22	0.47
1:A:565:MET:HE2	1:A:601:ASP:CB	2.44	0.47
1:A:548:ASN:O	1:A:551:LYS:HB3	2.13	0.47
1:A:575:ILE:O	1:A:579:ILE:HG12	2.15	0.47
1:A:769:ASP:HB3	1:A:773:MET:HE3	1.95	0.47
1:A:782:ALA:HA	1:A:785:PHE:CE2	2.49	0.47
1:A:309:ALA:CB	1:A:322:MET:HE1	2.44	0.47
1:A:551:LYS:HB2	1:A:551:LYS:HE3	1.64	0.47
1:A:689:ILE:HG21	1:A:732:LYS:HD3	1.96	0.47
1:A:482:THR:HA	1:A:490:PHE:O	2.15	0.47
1:A:3:LYS:HD2	1:A:3:LYS:HA	1.65	0.46
1:A:667:CYS:SG	1:A:717:VAL:HG21	2.55	0.46
1:A:148:PRO:O	1:A:149:LYS:C	2.57	0.46
1:A:295:GLU:HB2	1:A:302:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD12	1:A:184:LYS:HG3	1.97	0.46
1:A:744:ILE:HD13	1:A:763:PHE:HB3	1.97	0.46
1:A:37:PRO:HB3	1:A:241:THR:HG23	1.97	0.46
1:A:396:LEU:HD12	1:A:451:GLY:CA	2.44	0.46
1:A:519:GLY:O	1:A:520:SER:CB	2.63	0.46
1:A:707:LEU:HA	1:A:746:ILE:HD11	1.98	0.46
1:A:373:LEU:N	1:A:373:LEU:HD23	2.30	0.46
1:A:130:TYR:CD1	1:A:177:LYS:HA	2.51	0.46
1:A:537:ARG:HD3	1:A:851:TYR:CD1	2.51	0.46
1:A:722:VAL:HG23	1:A:740:ILE:CD1	2.45	0.46
1:A:419:GLU:C	1:A:421:GLY:H	2.24	0.46
1:A:521:PHE:CZ	1:A:525:MET:HG3	2.51	0.46
1:A:79:LYS:HB2	1:A:82:ASP:HB2	1.98	0.45
1:A:82:ASP:O	1:A:86:PRO:HB3	2.15	0.45
1:A:572:ILE:O	1:A:576:ARG:CG	2.64	0.45
1:A:148:PRO:C	1:A:150:SER:N	2.72	0.45
1:A:546:THR:HG23	1:A:557:ILE:HD11	1.99	0.45
1:A:685:MET:HE3	1:A:685:MET:HB3	1.87	0.45
1:A:122:LYS:O	1:A:122:LYS:HD3	2.17	0.45
1:A:148:PRO:O	1:A:150:SER:N	2.49	0.45
1:A:188:LYS:HA	1:A:194:GLU:O	2.16	0.45
1:A:552:LEU:HA	1:A:552:LEU:HD23	1.70	0.45
1:A:830:ILE:HB	1:A:849:LEU:CD2	2.47	0.45
1:A:102:MET:HG3	1:A:223:TYR:CD2	2.52	0.45
1:A:277:GLN:O	1:A:278:GLY:C	2.60	0.45
1:A:460:ALA:O	1:A:461:ARG:C	2.58	0.45
1:A:519:GLY:C	1:A:521:PHE:N	2.75	0.45
1:A:599:LYS:O	1:A:603:LYS:HG3	2.17	0.45
1:A:786:LEU:O	1:A:789:TYR:HB2	2.16	0.45
1:A:82:ASP:OD2	1:A:83:THR:N	2.50	0.45
1:A:468:VAL:HG22	1:A:503:GLY:HA2	1.99	0.45
1:A:271:GLU:HA	1:A:289:GLN:O	2.17	0.45
1:A:557:ILE:HD12	1:A:557:ILE:N	2.32	0.45
1:A:381:PHE:HZ	1:A:497:SER:HB3	1.81	0.44
1:A:797:SER:CB	1:A:802:ARG:HD3	2.47	0.44
1:A:244:PHE:HB3	1:A:246:ASN:OD1	2.18	0.44
1:A:436:ILE:HG23	1:A:437:GLU:H	1.80	0.44
1:A:483:PHE:CE1	1:A:490:PHE:HB2	2.53	0.44
1:A:165:VAL:HG12	1:A:166:HIS:N	2.33	0.44
1:A:618:TYR:CE1	1:A:703:ILE:HG23	2.53	0.44
1:A:424:VAL:CG1	1:A:425:ILE:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ALA:O	1:A:692:LYS:HB2	2.17	0.44
1:A:574:LYS:HD2	1:A:574:LYS:N	2.33	0.43
1:A:61:ILE:O	1:A:65:ILE:HG12	2.18	0.43
1:A:80:PHE:CE2	1:A:200:PRO:HB2	2.53	0.43
1:A:343:ALA:O	1:A:344:PRO:C	2.60	0.43
1:A:29:MET:HA	1:A:32:LEU:HD12	1.99	0.43
1:A:68:ALA:O	1:A:71:TRP:HB3	2.19	0.43
1:A:436:ILE:CG2	1:A:437:GLU:N	2.81	0.43
1:A:230:PRO:HD2	1:A:233:TRP:CE2	2.53	0.43
1:A:518:SER:O	1:A:521:PHE:CB	2.58	0.43
1:A:57:ILE:HD11	1:A:209:LYS:HG2	2.01	0.43
1:A:578:MET:HE1	1:A:676:ILE:HD11	2.01	0.43
1:A:707:LEU:CD2	1:A:746:ILE:HD11	2.48	0.43
1:A:830:ILE:HB	1:A:849:LEU:HD21	2.01	0.43
1:A:121:LYS:HA	1:A:121:LYS:HD3	1.56	0.43
1:A:162:GLU:C	1:A:164:GLY:N	2.67	0.43
1:A:199:GLU:O	1:A:200:PRO:C	2.61	0.43
1:A:398:ALA:HB1	1:A:457:ALA:CB	2.49	0.43
1:A:499:ASP:OD2	1:A:501:SER:HB2	2.19	0.43
1:A:579:ILE:CD1	1:A:623:LEU:HD13	2.49	0.43
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.66	0.43
1:A:327:GLU:O	1:A:328:GLU:C	2.61	0.43
1:A:42:VAL:HG21	1:A:65:ILE:HD12	2.01	0.42
1:A:188:LYS:HG3	1:A:194:GLU:O	2.20	0.42
1:A:565:MET:HE2	1:A:601:ASP:HB3	2.01	0.42
1:A:347:LEU:O	1:A:348:GLN:C	2.62	0.42
1:A:685:MET:O	1:A:689:ILE:HG12	2.19	0.42
1:A:85:ASP:OD1	1:A:122:LYS:HG3	2.19	0.42
1:A:623:LEU:HD23	1:A:623:LEU:HA	1.82	0.42
1:A:633:GLU:HA	1:A:636:GLU:HG3	2.02	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.82	0.42
1:A:399:SER:HA	1:A:400:PRO:HD2	1.84	0.42
1:A:717:VAL:O	1:A:721:VAL:HG23	2.20	0.42
1:A:173:ALA:O	1:A:177:LYS:HB2	2.20	0.42
1:A:460:ALA:HB1	1:A:465:THR:O	2.20	0.42
1:A:108:ASN:HB2	1:A:136:PHE:HB2	2.01	0.42
1:A:93:SER:HB3	1:A:211:VAL:HG13	2.02	0.41
1:A:99:MET:HG2	1:A:223:TYR:CE1	2.55	0.41
1:A:172:THR:HB	1:A:175:ASP:CG	2.45	0.41
1:A:243:VAL:HG11	1:A:332:TYR:CG	2.55	0.41
1:A:270:GLY:C	1:A:271:GLU:CG	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:HIS:CD2	1:A:845:HIS:C	2.98	0.41
1:A:7:LYS:HE2	1:A:71:TRP:CD1	2.55	0.41
1:A:284:GLY:HA2	1:A:288:PRO:HD3	2.02	0.41
1:A:765:PHE:CZ	1:A:816:VAL:HG23	2.55	0.41
1:A:514:GLU:HG2	1:A:515:ALA:N	2.35	0.41
1:A:563:GLU:CG	1:A:621:PRO:HD3	2.51	0.41
1:A:667:CYS:O	1:A:671:VAL:HG23	2.20	0.41
1:A:188:LYS:C	1:A:190:ALA:N	2.78	0.41
1:A:393:GLY:HA3	1:A:485:LEU:HD21	2.03	0.41
1:A:498:LEU:HD23	1:A:505:ILE:HG23	2.02	0.41
1:A:707:LEU:HA	1:A:746:ILE:HD13	2.01	0.41
1:A:165:VAL:CG1	1:A:166:HIS:N	2.83	0.41
1:A:342:THR:HB	1:A:344:PRO:HD2	2.02	0.41
1:A:350:ALA:O	1:A:354:VAL:HG23	2.21	0.41
1:A:557:ILE:O	1:A:557:ILE:HG22	2.19	0.41
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.84	0.41
1:A:763:PHE:CE2	1:A:826:LEU:HD21	2.55	0.41
1:A:427:VAL:HA	1:A:446:LEU:O	2.22	0.41
1:A:570:ASP:OD2	1:A:571:ARG:NE	2.53	0.41
1:A:674:PRO:O	1:A:678:LYS:HG3	2.21	0.41
1:A:399:SER:O	1:A:500:GLY:HA3	2.21	0.40
1:A:679:MET:C	1:A:679:MET:SD	3.04	0.40
1:A:689:ILE:HD13	1:A:736:MET:SD	2.61	0.40
1:A:491:ALA:O	1:A:492:GLU:C	2.64	0.40
1:A:521:PHE:CE2	1:A:525:MET:HG3	2.57	0.40
1:A:630:THR:HG22	1:A:632:GLU:N	2.34	0.40
1:A:3:LYS:HE2	1:A:5:VAL:O	2.22	0.40
1:A:134:ARG:C	1:A:134:ARG:HD2	2.46	0.40
1:A:603:LYS:NZ	1:A:690:GLU:OE1	2.48	0.40
1:A:429:LEU:HD11	1:A:449:ARG:HD3	2.03	0.40
1:A:859:VAL:N	1:A:860:PRO:CD	2.84	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	870/873 (100%)	820 (94%)	46 (5%)	4 (0%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	190	ALA
1	A	149	LYS
1	A	856	PRO

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	713/714 (100%)	673 (94%)	40 (6%)	19	24

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	31	ILE
1	A	98	SER
1	A	121	LYS
1	A	127	ARG
1	A	146	GLU
1	A	156	ILE
1	A	163	LYS
1	A	169	THR
1	A	192	ASN
1	A	213	ARG
1	A	216	ASP
1	A	222	VAL
1	A	268	ILE
1	A	279	GLU

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Mol	Chain	Res	Type
1	A	300	ASP
1	A	322	MET
1	A	334	LEU
1	A	373	LEU
1	A	436	ILE
1	A	458	VAL
1	A	473	GLU
1	A	476	ILE
1	A	488	HIS
1	A	505	ILE
1	A	513	GLN
1	A	517	VAL
1	A	520	SER
1	A	543	PRO
1	A	576	ARG
1	A	578	MET
1	A	607	LYS
1	A	617	ARG
1	A	636	GLU
1	A	698	ASP
1	A	743	MET
1	A	747	PRO
1	A	780	ASP
1	A	786	LEU
1	A	830	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	62	GLN
1	A	64	GLN
1	A	108	ASN
1	A	138	GLN
1	A	192	ASN
1	A	217	ASN
1	A	277	GLN
1	A	440	HIS
1	A	488	HIS
1	A	513	GLN
1	A	624	HIS
1	A	727	GLN

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Mol	Chain	Res	Type
1	A	845	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	SO4	A	1005	-	4,4,4	0.54	0	6,6,6	0.33	0
3	SO4	A	1004	-	4,4,4	0.45	0	6,6,6	0.17	0
4	PPR	A	1000	2	9,9,9	5.61	8 (88%)	12,13,13	2.90	6 (50%)
3	SO4	A	1003	-	4,4,4	1.39	1 (25%)	6,6,6	1.37	1 (16%)
3	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PPR	A	1000	2	-	3/8/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	PPR	P-C3	10.71	1.96	1.79
4	A	1000	PPR	C3-C2	-9.86	1.36	1.51
4	A	1000	PPR	O2-C2	4.37	1.32	1.23
4	A	1000	PPR	P-O2P	-4.12	1.45	1.55
4	A	1000	PPR	P-O3P	-3.14	1.47	1.55
4	A	1000	PPR	P-O1P	2.93	1.56	1.50
4	A	1000	PPR	O1-C1	2.89	1.29	1.22
4	A	1000	PPR	O2'-C1	-2.84	1.22	1.30
3	A	1003	SO4	O2-S	-2.02	1.32	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	PPR	O1-C1-C2	-5.16	115.40	121.81
4	A	1000	PPR	C3-C2-C1	4.92	130.30	118.00
4	A	1000	PPR	O2-C2-C1	-4.20	113.67	119.67
4	A	1000	PPR	O2'-C1-C2	3.29	122.72	113.59
4	A	1000	PPR	O3P-P-O2P	2.64	115.49	107.96
3	A	1003	SO4	O4-S-O3	2.60	122.88	108.54
4	A	1000	PPR	O2-C2-C3	-2.41	116.02	120.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1000	PPR	C2-C3-P-O2P
4	A	1000	PPR	C2-C3-P-O3P
4	A	1000	PPR	C2-C3-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	PPR	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, 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	872/873 (99%)	0.44	60 (6%) 23 20	3, 26, 60, 85	10 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	SER	5.5
1	A	488	HIS	4.6
1	A	478	GLU	4.3
1	A	165	VAL	4.2
1	A	150	SER	4.2
1	A	190	ALA	4.1
1	A	487	GLY	3.9
1	A	520	SER	3.9
1	A	167	PHE	3.8
1	A	192	ASN	3.7
1	A	516	SER	3.7
1	A	2	ALA	3.6
1	A	489	THR	3.5
1	A	514	GLU	3.5
1	A	189	GLU	3.4
1	A	630	THR	3.4
1	A	178	GLU	3.1
1	A	170	ASP	3.1
1	A	59	GLN	3.1
1	A	512	THR	3.1
1	A	662	MET	3.1
1	A	181	GLU	3.0
1	A	417	ALA	3.0
1	A	191	MET	3.0
1	A	385	ALA	3.0
1	A	420	LYS	3.0
1	A	515	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLU	2.9
1	A	148	PRO	2.8
1	A	169	THR	2.7
1	A	490	PHE	2.7
1	A	163	LYS	2.7
1	A	519	GLY	2.7
1	A	386	LEU	2.6
1	A	52	ASN	2.6
1	A	423	ARG	2.5
1	A	193	GLY	2.5
1	A	508	GLY	2.5
1	A	387	LYS	2.5
1	A	477	ASN	2.5
1	A	421	GLY	2.5
1	A	388	ALA	2.4
1	A	631	GLU	2.4
1	A	147	VAL	2.4
1	A	188	LYS	2.4
1	A	194	GLU	2.3
1	A	166	HIS	2.2
1	A	418	HIS	2.2
1	A	384	ALA	2.2
1	A	486	GLY	2.2
1	A	419	GLU	2.2
1	A	873	ASN	2.2
1	A	494	ASP	2.1
1	A	151	HIS	2.1
1	A	416	ALA	2.1
1	A	145	MET	2.1
1	A	641	MET	2.0
1	A	84	GLU	2.0
1	A	164	GLY	2.0
1	A	154	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1004	5/5	0.88	0.13	36,50,54,60	0
3	SO4	A	1005	5/5	0.94	0.17	20,39,49,53	0
4	PPR	A	1000	10/10	0.94	0.10	3,18,21,23	0
3	SO4	A	1003	5/5	0.96	0.16	2,16,19,20	5
2	MG	A	1001	1/1	0.96	0.06	7,7,7,7	0
3	SO4	A	1002	5/5	0.97	0.08	18,23,25,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.