



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:41 AM UTC

PDB ID : 2CUN / pdb\_00002cun  
Title : Crystal structure of Phosphoglycerate Kinase from *Pyrococcus horikoshii* OT3  
Authors : Mizutani, H.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2005-05-27  
Resolution : 2.10 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](mailto: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>.

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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

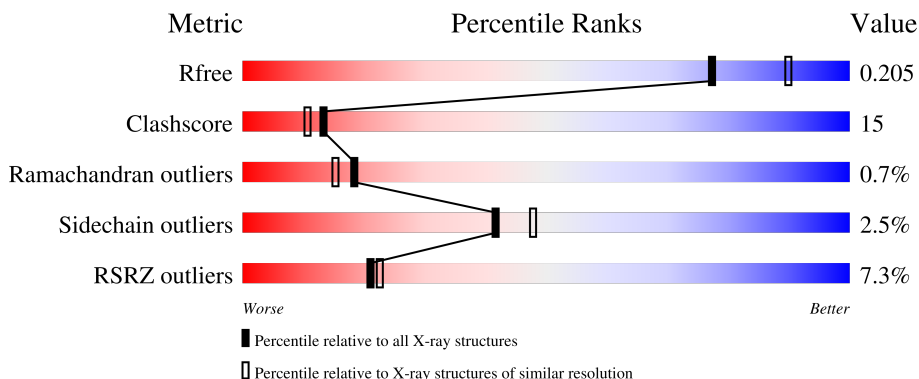
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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  $\geq 3$ , 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	410	 75% 22% ..
1	B	410	 13% 62% 35% ..

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
3	3PG	A	503	-	X	-	-
3	3PG	B	504	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6890 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.

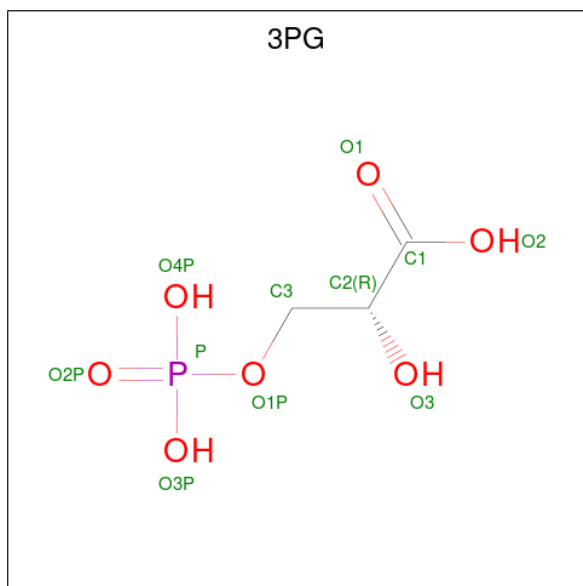
- Molecule 1 is a protein called Phosphoglycerate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	Total 3229	C 2078	N 544	O 595	S 12	0	0	0
1	B	405	Total 3230	C 2078	N 544	O 596	S 12	0	1	0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total 1	Cl 1	0
2	B	1	Total 1	Cl 1	0

- Molecule 3 is 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



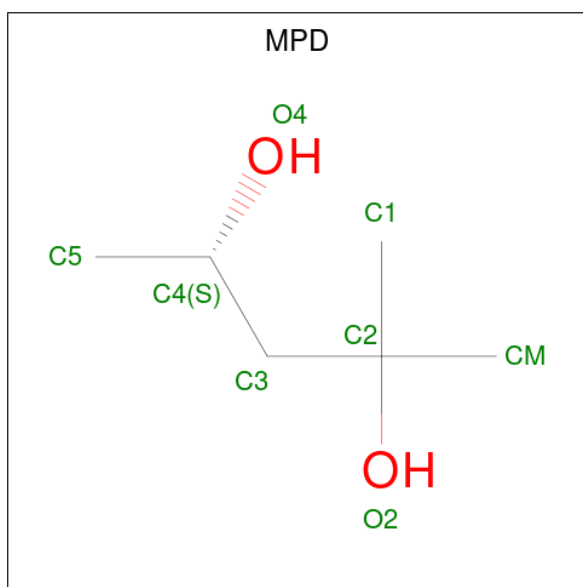
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	3	7	1		
3	B	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0

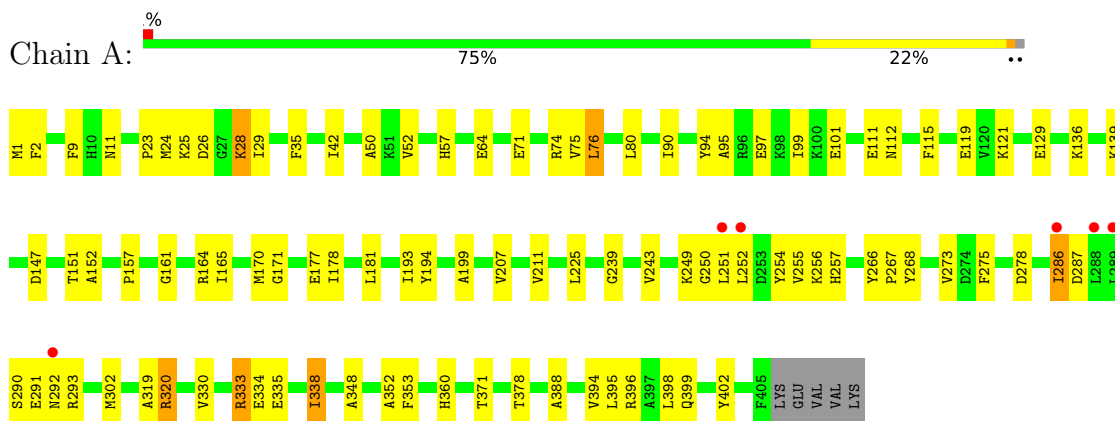
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	218	Total O 218 218	0	0
6	B	153	Total O 153 153	0	0

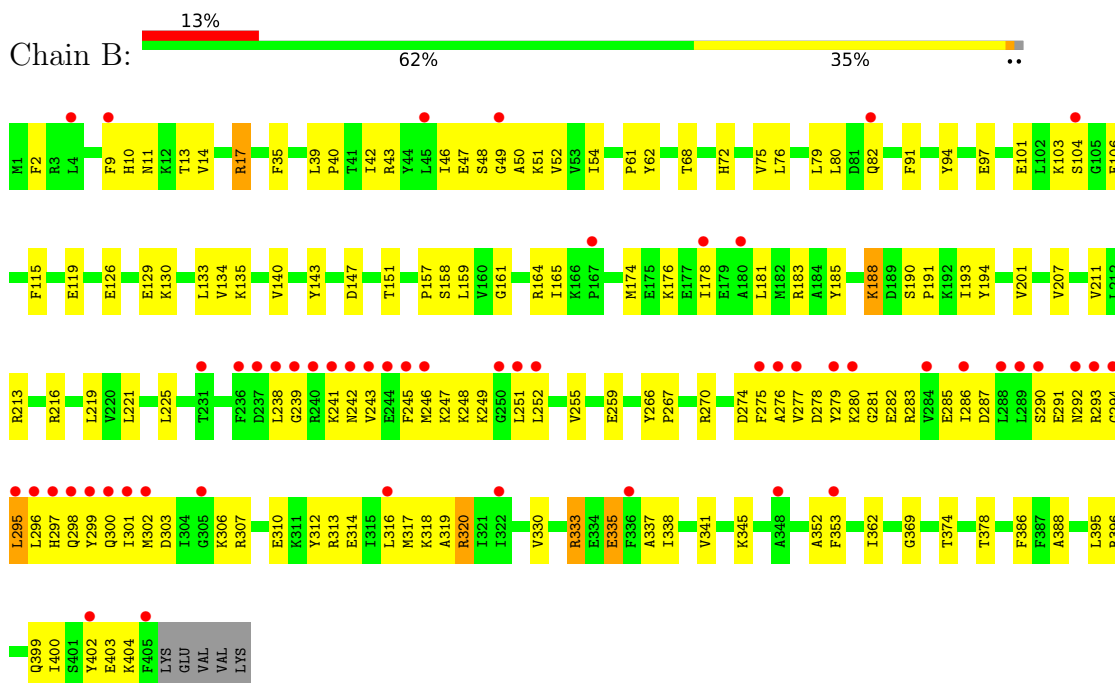
### 3 Residue-property plots

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: Phosphoglycerate kinase



- Molecule 1: Phosphoglycerate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.85Å 123.33Å 82.94Å 90.00° 95.42° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.10) 99.9 (30.00-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.244 0.212 , 0.205	Depositor DCC
$R_{free}$ test set	2945 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtrriage
Anisotropy	0.493	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, 3PG, CL, GOL

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	0.39	0/3289	0.91	10/4423 (0.2%)
1	B	0.36	0/3295	0.89	9/4431 (0.2%)
All	All	0.38	0/6584	0.90	19/8854 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	PHE	N-CA-C	-9.50	101.69	113.28
1	A	115	PHE	N-CA-C	-9.25	101.76	113.23
1	A	353	PHE	N-CA-C	-7.61	97.61	109.25
1	A	52	VAL	N-CA-C	6.53	117.52	107.99
1	A	161	GLY	N-CA-C	5.88	120.94	113.24
1	B	320	ARG	N-CA-C	-5.78	106.58	113.97
1	B	388	ALA	N-CA-C	-5.68	106.11	113.16
1	A	320	ARG	N-CA-C	-5.67	106.49	113.41
1	B	378	THR	N-CA-C	-5.66	106.21	113.23
1	B	161	GLY	N-CA-C	5.65	120.64	113.24
1	B	52	VAL	N-CA-C	5.58	116.76	108.23
1	A	388	ALA	N-CA-C	-5.47	106.60	113.28
1	A	273	VAL	N-CA-C	-5.42	106.56	113.22
1	B	201	VAL	N-CA-C	5.37	115.51	110.30
1	B	193	ILE	N-CA-C	5.37	115.83	107.99
1	A	193	ILE	N-CA-C	5.36	115.67	108.17
1	A	378	THR	N-CA-C	-5.29	106.83	113.28
1	A	171	GLY	N-CA-C	-5.21	104.62	112.60
1	B	68	THR	N-CA-C	-5.06	104.18	110.41

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	3229	0	3292	79	0
1	B	3230	0	3293	116	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	11	0	4	0	0
3	B	11	0	4	0	0
4	A	6	0	8	2	0
4	B	6	0	8	0	0
5	A	16	0	28	1	0
5	B	8	0	14	1	0
6	A	218	0	0	6	0
6	B	153	0	0	2	0
All	All	6890	0	6651	195	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 15.

All (195) 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:188:LYS:HD3	1:B:188:LYS:H	1.34	0.92
1:A:338:ILE:HD12	1:A:338:ILE:H	1.33	0.92
1:B:333:ARG:HH11	1:B:333:ARG:HB3	1.42	0.85
1:A:35:PHE:HD1	1:A:76:LEU:HD13	1.43	0.83
1:A:178:ILE:HD12	1:A:395:LEU:HD21	1.61	0.82
1:B:119:GLU:HA	1:B:157:PRO:HG2	1.64	0.79
1:A:136:LYS:HA	1:A:139:LYS:HE3	1.65	0.77
1:B:247:LYS:HG2	1:B:252:LEU:HD12	1.65	0.77
1:B:318:LYS:HA	1:B:318:LYS:HE2	1.67	0.77
1:B:188:LYS:HD3	1:B:188:LYS:N	2.00	0.76
1:A:396:ARG:HA	1:A:399:GLN:HE21	1.52	0.74
1:B:296:LEU:H	1:B:296:LEU:HD12	1.50	0.74
1:B:319:ALA:O	1:B:352:ALA:HB2	1.88	0.73
1:A:249:LYS:HB3	1:A:251:LEU:HD13	1.71	0.73
1:A:24:MET:HE3	1:A:29:ILE:HG13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:HD2	1:B:158:SER:OG	1.91	0.70
1:B:245:PHE:O	1:B:248:LYS:HB2	1.91	0.70
1:B:287:ASP:OD2	1:B:307:ARG:HD3	1.90	0.70
1:A:333:ARG:HH11	1:A:333:ARG:HB3	1.56	0.70
1:B:225:LEU:HD13	1:B:251:LEU:HD21	1.73	0.69
1:A:338:ILE:H	1:A:338:ILE:CD1	2.05	0.69
1:B:306:LYS:O	1:B:310:GLU:HG3	1.93	0.69
1:B:302:MET:HE2	1:B:330:VAL:HG21	1.74	0.69
1:B:313:ARG:O	1:B:317:MET:HG2	1.93	0.68
1:B:188:LYS:H	1:B:188:LYS:CD	2.05	0.68
1:A:97:GLU:O	1:A:101:GLU:HG3	1.94	0.67
1:A:129:GLU:OE1	1:A:164:ARG:HD2	1.93	0.67
1:A:338:ILE:HD12	1:A:338:ILE:N	2.10	0.66
1:A:35:PHE:CD1	1:A:76:LEU:HD13	2.29	0.66
1:B:255:VAL:O	1:B:259:GLU:HG3	1.96	0.66
1:A:250:GLY:HA2	6:A:666:HOH:O	1.97	0.65
1:B:14:VAL:HG22	1:B:143:TYR:HB2	1.78	0.64
1:B:306:LYS:HE3	1:B:310:GLU:OE1	1.98	0.63
1:B:293:ARG:HH11	1:B:293:ARG:HB2	1.63	0.63
1:B:287:ASP:HB3	1:B:290:SER:HB2	1.80	0.63
1:A:119:GLU:HA	1:A:157:PRO:HG2	1.82	0.61
1:B:54:ILE:HD13	1:B:76:LEU:HD21	1.81	0.61
1:B:241:LYS:HB3	1:B:299:TYR:O	2.00	0.61
1:A:256:LYS:HG3	1:A:257:HIS:H	1.65	0.60
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.65	0.60
1:A:178:ILE:CD1	1:A:395:LEU:HD21	2.30	0.59
1:B:97:GLU:O	1:B:101:GLU:HG3	2.01	0.59
1:A:335:GLU:H	1:A:335:GLU:CD	2.10	0.59
1:B:296:LEU:H	1:B:296:LEU:CD1	2.15	0.59
1:B:337:ALA:O	1:B:341:VAL:HG23	2.03	0.59
1:A:29:ILE:HG13	1:A:71:GLU:OE1	2.03	0.59
1:A:23:PRO:HG3	1:A:360:HIS:CG	2.38	0.59
1:B:320:ARG:HH11	1:B:320:ARG:HG3	1.68	0.59
1:A:9:PHE:HB3	1:A:50:ALA:HB2	1.84	0.58
1:B:296:LEU:HD12	1:B:296:LEU:N	2.17	0.58
1:B:280:LYS:O	1:B:280:LYS:HG2	2.03	0.58
1:B:252:LEU:HA	1:B:255:VAL:HG23	1.86	0.58
1:A:267:PRO:HG2	1:A:268:TYR:CD1	2.39	0.57
1:A:24:MET:HE3	1:A:29:ILE:CG1	2.34	0.57
1:A:286:ILE:H	1:A:286:ILE:HD13	1.69	0.57
1:B:239:GLY:O	1:B:243:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:HB2	1:A:286:ILE:HD11	1.86	0.57
1:B:310:GLU:O	1:B:314:GLU:HG3	2.05	0.57
1:B:295:LEU:HD22	1:B:299:TYR:CE2	2.40	0.56
1:B:42:ILE:O	1:B:46:ILE:HG13	2.05	0.56
1:B:130:LYS:HA	1:B:135:LYS:HE3	1.86	0.56
1:B:335:GLU:H	1:B:335:GLU:CD	2.12	0.56
1:B:75:VAL:O	1:B:79:LEU:HD13	2.06	0.56
1:B:35:PHE:HD1	1:B:76:LEU:HD13	1.71	0.56
1:B:129:GLU:OE1	1:B:164:ARG:HD2	2.06	0.56
1:B:239:GLY:HA3	1:B:296:LEU:HB3	1.87	0.56
1:A:1:MET:HE3	1:A:398:LEU:HD13	1.88	0.55
1:B:2:PHE:CE1	1:B:402:TYR:HA	2.41	0.55
1:A:74:ARG:HG3	1:A:75:VAL:N	2.22	0.55
1:A:252:LEU:HA	1:A:255:VAL:HG23	1.88	0.55
1:A:287:ASP:HB3	1:A:290:SER:CB	2.37	0.54
1:A:239:GLY:O	1:A:243:VAL:HG23	2.08	0.54
1:B:341:VAL:HG12	1:B:345:LYS:HE3	1.89	0.54
1:B:126:GLU:H	1:B:126:GLU:CD	2.16	0.54
1:A:333:ARG:HB3	1:A:333:ARG:NH1	2.23	0.54
1:B:277:VAL:HG22	1:B:278:ASP:N	2.23	0.54
1:B:362:ILE:HG13	5:B:507:MPD:HM1	1.90	0.54
1:A:287:ASP:HB3	1:A:290:SER:HB2	1.90	0.53
1:B:242:ASN:O	1:B:246:MET:HG2	2.08	0.53
1:B:43:ARG:O	1:B:47:GLU:HG2	2.09	0.53
1:B:17:ARG:HD3	1:B:159:LEU:HD23	1.90	0.53
1:B:213:ARG:HG3	6:B:635:HOH:O	2.09	0.53
1:B:395:LEU:O	1:B:399:GLN:HG3	2.09	0.53
1:B:292:ASN:C	1:B:293:ARG:HG3	2.34	0.52
1:B:293:ARG:HH11	1:B:293:ARG:CB	2.21	0.52
1:A:28:LYS:HB3	1:A:28:LYS:NZ	2.24	0.52
1:B:396:ARG:O	1:B:400:ILE:HG13	2.09	0.52
1:B:10:HIS:HA	1:B:48:SER:O	2.09	0.52
1:B:292:ASN:O	1:B:293:ARG:HG3	2.10	0.52
1:A:256:LYS:HG3	1:A:257:HIS:N	2.25	0.52
1:A:178:ILE:HD11	1:A:395:LEU:HD11	1.92	0.51
1:B:9:PHE:HB3	1:B:50:ALA:HB2	1.93	0.51
1:B:249:LYS:HB2	1:B:251:LEU:HD13	1.91	0.51
1:B:295:LEU:HB3	1:B:299:TYR:HD2	1.76	0.51
1:A:293:ARG:HH11	1:A:293:ARG:HG3	1.76	0.51
1:B:207:VAL:O	1:B:211:VAL:HG22	2.11	0.51
1:B:276:ALA:HA	1:B:285:GLU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:LYS:HG2	1:B:106:GLU:OE1	2.11	0.51
1:A:94:TYR:HB2	1:B:94:TYR:HB2	1.93	0.51
1:A:121:LYS:NZ	6:A:633:HOH:O	2.44	0.51
1:A:278:ASP:HB2	1:A:302:MET:HG3	1.92	0.50
1:B:238:LEU:O	1:B:242:ASN:HB2	2.11	0.50
1:B:183:ARG:HD3	1:B:353:PHE:CE2	2.47	0.50
1:A:348:ALA:HB1	1:A:371:THR:O	2.12	0.50
1:A:225:LEU:HD13	1:A:251:LEU:HD21	1.93	0.50
1:A:291:GLU:C	1:A:293:ARG:H	2.20	0.50
1:A:64:GLU:HG2	6:A:707:HOH:O	2.11	0.50
1:A:319:ALA:O	1:A:352:ALA:HB2	2.12	0.50
1:B:402:TYR:C	1:B:404:LYS:H	2.20	0.49
1:A:119:GLU:HA	1:A:157:PRO:CG	2.43	0.49
1:B:275:PHE:HD2	1:B:301:ILE:HG21	1.77	0.49
1:A:2:PHE:CE1	1:A:402:TYR:HA	2.48	0.49
1:B:221:LEU:HD23	1:B:270:ARG:HB2	1.95	0.48
1:B:333:ARG:HH11	1:B:333:ARG:CB	2.19	0.48
1:B:295:LEU:HB3	1:B:299:TYR:CD2	2.48	0.48
1:A:177:GLU:O	1:A:181:LEU:HD13	2.13	0.48
1:A:207:VAL:O	1:A:211:VAL:HG22	2.14	0.48
1:A:194:TYR:CE2	1:A:211:VAL:HG11	2.48	0.48
1:B:190:SER:HB2	1:B:191:PRO:HA	1.96	0.48
1:B:225:LEU:HD13	1:B:251:LEU:CD2	2.42	0.48
1:A:266:TYR:N	1:A:267:PRO:HD2	2.29	0.47
1:B:294:GLY:O	1:B:296:LEU:N	2.47	0.47
1:B:247:LYS:CG	1:B:252:LEU:HD12	2.40	0.47
1:A:396:ARG:HA	1:A:399:GLN:NE2	2.24	0.47
1:A:249:LYS:CB	1:A:251:LEU:HD13	2.43	0.47
1:B:183:ARG:HD3	1:B:353:PHE:CZ	2.49	0.47
1:B:190:SER:O	1:B:320:ARG:HG3	2.15	0.47
1:B:13:THR:HG21	1:B:140:VAL:O	2.14	0.47
1:B:279:TYR:O	1:B:280:LYS:HB3	2.15	0.46
1:A:199:ALA:CB	1:A:225:LEU:HD12	2.45	0.46
1:B:80:LEU:C	1:B:82:GLN:H	2.24	0.46
1:A:330:VAL:CG1	1:A:333:ARG:HG3	2.45	0.46
1:B:13:THR:HA	1:B:51:LYS:HB2	1.97	0.46
1:B:266:TYR:N	1:B:267:PRO:HD2	2.30	0.46
1:A:1:MET:HE2	1:A:170:MET:SD	2.56	0.46
1:B:103:LYS:HB2	1:B:106:GLU:HG3	1.96	0.46
1:B:181:LEU:HB3	1:B:386:PHE:CE2	2.51	0.46
1:A:275:PHE:O	1:A:286:ILE:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:505:CL:CL	4:A:501:GOL:O1	2.68	0.46
1:B:312:TYR:O	1:B:316:LEU:HG	2.16	0.46
1:A:152:ALA:HA	1:A:394:VAL:CG2	2.46	0.46
1:B:49:GLY:O	1:B:104:SER:HB2	2.15	0.45
1:B:277:VAL:HG23	1:B:300:GLN:O	2.15	0.45
1:B:134:VAL:CG1	1:B:165:ILE:HD12	2.47	0.45
1:B:133:LEU:C	1:B:133:LEU:HD23	2.42	0.45
1:A:95:ALA:O	1:A:99:ILE:HG13	2.17	0.45
1:A:291:GLU:C	1:A:293:ARG:N	2.75	0.45
1:B:276:ALA:HB2	1:B:285:GLU:HG2	1.99	0.44
1:B:61:PRO:O	1:B:62:TYR:HB2	2.16	0.44
1:B:185:TYR:O	1:B:216:ARG:HD2	2.18	0.44
1:B:353:PHE:CD1	1:B:374:THR:HG21	2.52	0.44
1:B:287:ASP:HB3	1:B:290:SER:CB	2.46	0.44
1:A:57:HIS:HE2	4:A:501:GOL:H11	1.83	0.44
1:B:294:GLY:C	1:B:296:LEU:N	2.76	0.44
1:B:126:GLU:O	1:B:130:LYS:HD3	2.17	0.43
1:A:25:LYS:HD2	1:A:26:ASP:OD2	2.18	0.43
1:A:333:ARG:NH1	1:A:335:GLU:OE2	2.51	0.43
1:A:330:VAL:HG11	1:A:333:ARG:HG3	2.01	0.43
1:B:341:VAL:CG1	1:B:345:LYS:HE3	2.47	0.43
1:B:302:MET:O	1:B:303:ASP:HB2	2.19	0.43
1:A:249:LYS:C	1:A:251:LEU:H	2.27	0.43
1:A:293:ARG:NE	6:A:570:HOH:O	2.52	0.43
1:A:28:LYS:HB3	1:A:28:LYS:HZ3	1.84	0.43
1:B:277:VAL:CG2	1:B:278:ASP:N	2.82	0.43
1:A:1:MET:CE	1:A:398:LEU:HD13	2.49	0.42
1:A:42:ILE:HG21	1:A:80:LEU:HD11	2.01	0.42
1:B:341:VAL:O	1:B:345:LYS:HG3	2.18	0.42
1:B:119:GLU:HA	1:B:157:PRO:CG	2.42	0.42
1:A:139:LYS:HE2	6:A:563:HOH:O	2.19	0.42
1:B:293:ARG:CB	1:B:293:ARG:NH1	2.83	0.42
1:B:43:ARG:HG3	1:B:43:ARG:NH1	2.33	0.42
1:B:286:ILE:HG21	1:B:293:ARG:HG2	2.02	0.42
1:B:353:PHE:HD1	1:B:374:THR:HG21	1.84	0.42
1:A:320:ARG:HD3	1:A:320:ARG:HA	1.86	0.42
1:A:24:MET:HE2	1:A:28:LYS:C	2.44	0.42
1:A:136:LYS:HA	1:A:139:LYS:CE	2.44	0.42
1:A:1:MET:HE3	1:A:398:LEU:CB	2.50	0.41
1:B:279:TYR:C	1:B:281:GLY:H	2.27	0.41
1:B:283:ARG:NE	1:B:338:ILE:HD12	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HG3	1:B:320:ARG:NH1	2.34	0.41
1:A:252:LEU:C	1:A:254:TYR:H	2.29	0.41
1:B:274:ASP:HB2	1:B:286:ILE:O	2.21	0.41
1:A:1:MET:HE3	1:A:398:LEU:HB3	2.02	0.41
1:A:90:ILE:HD12	5:A:509:MPD:CM	2.51	0.41
1:B:39:LEU:HB2	1:B:40:PRO:HD3	2.03	0.41
1:B:72:HIS:O	1:B:76:LEU:HB2	2.21	0.41
1:B:91:PHE:CD2	1:B:133:LEU:HA	2.56	0.41
1:B:194:TYR:CE2	1:B:211:VAL:HG11	2.55	0.41
1:B:219:LEU:HD11	1:B:270:ARG:NH1	2.36	0.41
1:B:176:LYS:HG3	6:B:589:HOH:O	2.20	0.41
1:A:111:GLU:HG3	1:A:112:ASN:N	2.36	0.40
1:B:174:MET:O	1:B:178:ILE:HG13	2.21	0.40
1:B:320:ARG:C	1:B:352:ALA:HB1	2.47	0.40
1:A:129:GLU:HB2	1:A:165:ILE:HD11	2.04	0.40
1:A:334:GLU:HG2	6:A:681:HOH:O	2.21	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	403/410 (98%)	392 (97%)	10 (2%)	1 (0%)	43	44
1	B	404/410 (98%)	375 (93%)	24 (6%)	5 (1%)	10	7
All	All	807/820 (98%)	767 (95%)	34 (4%)	6 (1%)	18	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	LEU
1	B	298	GLN

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Mol	Chain	Res	Type
1	B	369	GLY
1	A	292	ASN
1	B	291	GLU
1	B	403	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/350 (99%)	337 (98%)	8 (2%)	44	51
1	B	346/350 (99%)	337 (97%)	9 (3%)	40	46
All	All	691/700 (99%)	674 (98%)	17 (2%)	42	48

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	28	LYS
1	A	76	LEU
1	A	147	ASP
1	A	151	THR
1	A	286	ILE
1	A	333	ARG
1	A	338	ILE
1	B	11	ASN
1	B	17	ARG
1	B	147	ASP
1	B	151	THR
1	B	188	LYS
1	B	282	GLU
1	B	297	HIS
1	B	333	ARG
1	B	335	GLU

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	82	GLN
1	A	83	HIS
1	A	399	GLN
1	B	298	GLN

### 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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	GOL	B	502	-	5,5,5	0.26	0	5,5,5	0.33	0
5	MPD	B	507	-	7,7,7	0.59	0	9,10,10	0.33	0
3	3PG	B	504	-	9,10,10	3.39	5 (55%)	11,14,14	2.50	3 (27%)
4	GOL	A	501	-	5,5,5	0.28	0	5,5,5	0.39	0
5	MPD	A	508	-	7,7,7	0.57	0	9,10,10	0.35	0
3	3PG	A	503	-	9,10,10	3.45	6 (66%)	11,14,14	2.55	3 (27%)
5	MPD	A	509	-	7,7,7	0.73	0	9,10,10	0.38	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	GOL	B	502	-	-	0/4/4/4	-
5	MPD	B	507	-	-	0/5/5/5	-
3	3PG	B	504	-	-	6/10/10/10	-
4	GOL	A	501	-	-	0/4/4/4	-
5	MPD	A	508	-	-	0/5/5/5	-
3	3PG	A	503	-	-	6/10/10/10	-
5	MPD	A	509	-	-	0/5/5/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	3PG	P-O2P	5.92	1.68	1.50
3	B	504	3PG	P-O2P	5.86	1.68	1.50
3	B	504	3PG	O1-C1	5.01	1.36	1.22
3	A	503	3PG	O1-C1	4.97	1.36	1.22
3	A	503	3PG	P-O4P	3.96	1.69	1.54
3	A	503	3PG	P-O3P	3.72	1.68	1.54
3	B	504	3PG	P-O4P	3.65	1.68	1.54
3	B	504	3PG	P-O3P	3.48	1.67	1.54
3	B	504	3PG	C2-C1	-3.24	1.47	1.52
3	A	503	3PG	C2-C1	-3.16	1.47	1.52
3	A	503	3PG	P-O1P	2.02	1.66	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	3PG	O2-C1-C2	6.25	125.95	112.74
3	B	504	3PG	O2-C1-C2	6.18	125.81	112.74
3	A	503	3PG	O2-C1-O1	-4.17	114.62	124.08
3	B	504	3PG	O2-C1-O1	-4.16	114.64	124.08
3	B	504	3PG	O1P-C3-C2	2.09	113.85	107.96
3	A	503	3PG	O1P-C3-C2	2.07	113.79	107.96

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	3PG	O1-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
3	B	504	3PG	O2-C1-C2-O3
3	B	504	3PG	C1-C2-C3-O1P
3	A	503	3PG	C1-C2-C3-O1P
3	A	503	3PG	O2-C1-C2-O3
3	A	503	3PG	O3-C2-C3-O1P
3	B	504	3PG	O3-C2-C3-O1P
3	A	503	3PG	O1-C1-C2-O3
3	B	504	3PG	O1-C1-C2-C3
3	B	504	3PG	O2-C1-C2-C3
3	A	503	3PG	O1-C1-C2-C3
3	A	503	3PG	O2-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	507	MPD	1	0
4	A	501	GOL	2	0
5	A	509	MPD	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/410 (98%)	-0.06	6 (1%) 72 74	22, 36, 60, 78	0
1	B	405/410 (98%)	0.68	53 (13%) 7 7	22, 46, 81, 93	1 (0%)
All	All	810/820 (98%)	0.31	59 (7%) 21 22	22, 40, 72, 93	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	LEU	5.8
1	B	286	ILE	4.9
1	B	405	PHE	4.6
1	B	299	TYR	4.3
1	B	237	ASP	3.9
1	B	295	LEU	3.9
1	B	297	HIS	3.8
1	B	289	LEU	3.7
1	B	288	LEU	3.7
1	B	284	VAL	3.5
1	B	279	TYR	3.4
1	B	294	GLY	3.4
1	B	245	PHE	3.4
1	A	288	LEU	3.1
1	B	236	PHE	3.0
1	B	243	VAL	3.0
1	B	293	ARG	3.0
1	B	240	ARG	3.0
1	B	292	ASN	2.9
1	B	277	VAL	2.9
1	B	298	GLN	2.8
1	B	238	LEU	2.8
1	B	252	LEU	2.8
1	B	275	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	241	LYS	2.7
1	B	353	PHE	2.6
1	B	244	GLU	2.6
1	B	301	ILE	2.6
1	A	252	LEU	2.5
1	B	4	LEU	2.5
1	B	178	ILE	2.5
1	B	242	ASN	2.5
1	B	45	LEU	2.4
1	B	402	TYR	2.4
1	B	336	PHE	2.4
1	B	9	PHE	2.3
1	B	104	SER	2.3
1	B	231	THR	2.3
1	B	316	LEU	2.3
1	B	290	SER	2.3
1	A	286	ILE	2.3
1	B	250	GLY	2.3
1	B	348	ALA	2.2
1	B	251	LEU	2.2
1	B	276	ALA	2.2
1	B	246	MET	2.2
1	B	180	ALA	2.2
1	B	300	GLN	2.1
1	A	289	LEU	2.1
1	B	322	ILE	2.1
1	A	292	ASN	2.1
1	B	302	MET	2.1
1	B	49	GLY	2.1
1	B	239	GLY	2.1
1	B	280	LYS	2.1
1	B	167	PRO	2.1
1	A	251	LEU	2.0
1	B	82	GLN	2.0
1	B	305	GLY	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	MPD	A	509	8/8	0.83	0.18	31,42,46,49	0
2	CL	B	506	1/1	0.87	0.14	68,68,68,68	0
5	MPD	B	507	8/8	0.87	0.14	42,44,45,45	0
5	MPD	A	508	8/8	0.88	0.13	41,45,46,46	0
4	GOL	A	501	6/6	0.89	0.12	39,47,51,54	0
4	GOL	B	502	6/6	0.92	0.10	33,40,43,46	0
2	CL	A	505	1/1	0.92	0.12	64,64,64,64	0
3	3PG	A	503	11/11	0.93	0.10	58,63,69,70	0
3	3PG	B	504	11/11	0.95	0.10	37,47,59,60	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.