



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1KC7  
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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

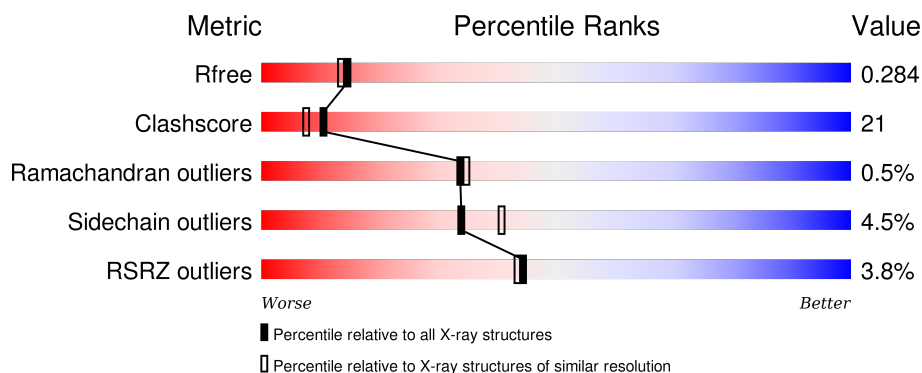
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	

## 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



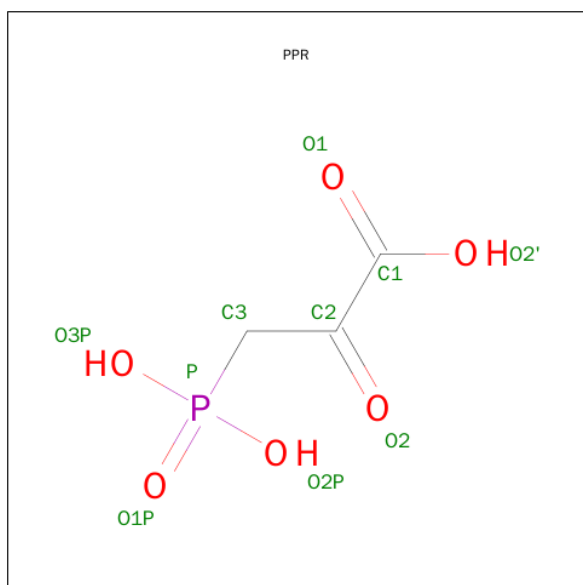
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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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 (three-letter code: PPR) (formula:  $C_3H_5O_6P$ ).

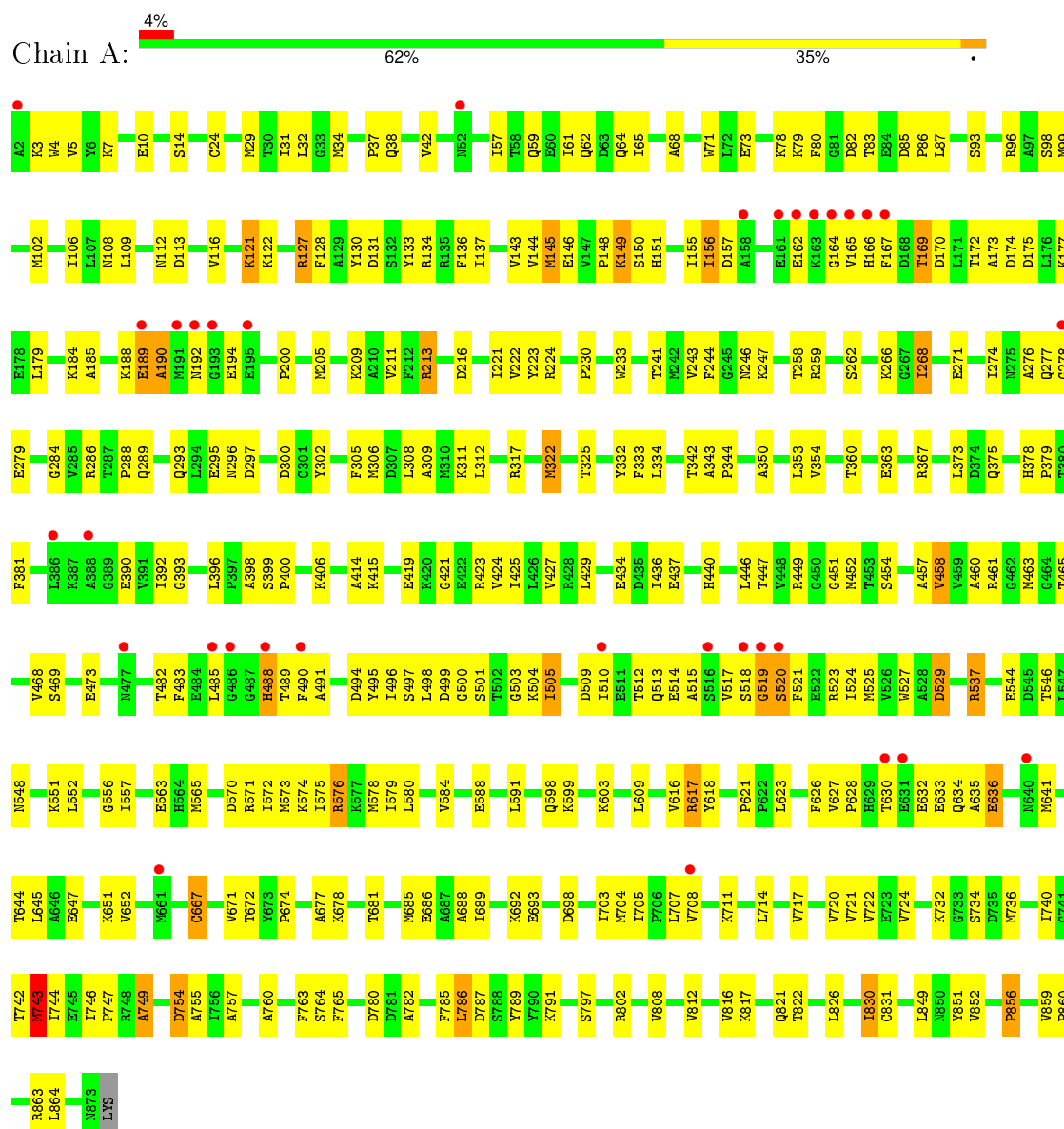


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		

### 3 Residue-property plots

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.

- Molecule 1: pyruvate phosphate dikinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.21Å 58.42Å 102.55Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 36.17 – 1.73	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.00-2.20) 90.0 (36.17-1.73)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 1.73Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.198 , 0.269 0.241 , 0.284	Depositor DCC
$R_{free}$ test set	2607 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 104444 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: PPR, MG, 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	0.79	5/6876 (0.1%)	0.91	9/9269 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	812	VAL	CB-CG2	7.08	1.67	1.52
1	A	616	VAL	CB-CG1	6.42	1.66	1.52
1	A	749	ALA	CA-CB	-5.55	1.40	1.52
1	A	544	GLU	CG-CD	5.18	1.59	1.51
1	A	667	CYS	CB-SG	-5.12	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	A	537	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	519	GLY	N-CA-C	-6.94	95.75	113.10
1	A	617	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	529	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	743	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	754	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	145	MET	N-CA-C	-5.04	97.38	111.00
1	A	127	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	6752	0	6668	285	0
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	285	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 21.

All (285) 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:396:LEU:HB3	1:A:452:MET:HE3	1.28	1.15
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:312:LEU:HD12	1:A:322:MET:HE2	1.32	1.08
1:A:396:LEU:HB3	1:A:452:MET:CE	1.84	1.06
1:A:557:ILE:HD13	1:A:609:LEU:HD21	1.50	0.94
1:A:172:THR:HG22	1:A:174:ASP:N	1.83	0.92
1:A:106:ILE:HD11	1:A:143:VAL:HG11	1.51	0.90
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:309:ALA:HA	1:A:322:MET:HE3	1.62	0.81
1:A:579:ILE:CD1	1:A:623:LEU:HD22	2.08	0.80
1:A:156:ILE:HG13	1:A:179:LEU:HD21	1.65	0.79
1:A:360:THR:OG1	1:A:363:GLU:HG3	1.84	0.77
1:A:165:VAL:HG13	1:A:170:ASP:HB2	1.68	0.76
1:A:529:ASP:CG	1:A:863:ARG:HH21	1.90	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:678:LYS:HG2	1:A:720:VAL:CG1	2.17	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:GLY:C	1:A:557:ILE:HD12	2.09	0.73
1:A:743:MET:C	1:A:744:ILE:HD12	2.09	0.72
1:A:440:HIS:HB2	1:A:463:MET:HE2	1.71	0.71
1:A:317:ARG:HH22	1:A:363:GLU:CD	1.94	0.70
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:HD12	1:A:505:ILE:N	2.06	0.70
1:A:4:TRP:H	1:A:64:GLN:HE22	1.40	0.70
1:A:580:LEU:HD23	1:A:651:LYS:HG2	1.75	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: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:N	1:A:705:ILE:HD12	2.11	0.66
1:A:268:ILE:HD11	1:A:305:PHE:HE2	1.60	0.66
1:A:32:LEU:HD22	1:A:311:LYS:NZ	2.09	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: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:309:ALA:HA	1:A:322:MET:HE1	1.78	0.64
1:A:80:PHE:HA	1:A:87:LEU:HB3	1.79	0.64
1:A:482:THR:HG22	1:A:491:ALA:HA	1.80	0.63
1:A:96:ARG:HD2	1:A:233:TRP:CZ3	2.34	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: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:N	1:A:434:GLU:OE1	2.21	0.62
1:A:65:ILE:HG21	1:A:205:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:520:SER:HA	1:A:523:ARG:HB2	1.83	0.59
1:A:744:ILE:N	1:A:744:ILE:HD12	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:162:GLU:C	1:A:164:GLY:H	2.05	0.58
1:A:689:ILE:O	1:A:693:GLU:HG3	2.02	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:156:ILE:HG13	1:A:179:LEU:CD2	2.34	0.58
1:A:131:ASP:O	1:A:134:ARG:HG3	2.03	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:65:ILE:HG21	1:A:205:MET:CE	2.34	0.58
1:A:38:GLN:O	1:A:241:THR:HG22	2.04	0.57
1:A:742:THR:HG23	1:A:744:ILE:HD11	1.87	0.57
1:A:488:HIS:CG	1:A:489:THR:H	2.22	0.57
1:A:644:THR:OG1	1:A:647:GLU:HG3	2.05	0.57
1:A:632:GLU:O	1:A:635:ALA:HB3	2.05	0.57
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:354:VAL:HG21	1:A:527:TRP:CZ3	2.41	0.56
1:A:293:GLN:O	1:A:296:ASN:HB2	2.05	0.56
1:A:514:GLU:HG2	1:A:515:ALA:O	2.05	0.56
1:A:454:SER:O	1:A:458:VAL:HG13	2.05	0.56
1:A:390:GLU:O	1:A:392:ILE:HG23	2.06	0.56
1:A:259:ARG:NH1	1:A:266:LYS:HG3	2.21	0.56
1:A:130:TYR:CZ	1:A:177:LYS:HG3	2.41	0.56
1:A:520:SER:O	1:A:524:ILE:HG12	2.06	0.56
1:A:185:ALA:O	1:A:189:GLU:HB3	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:584:VAL:O	1:A:588:GLU:HG3	2.06	0.55
1:A:128:PHE:CZ	1:A:247:LYS:HG3	2.42	0.55
1:A:78:LYS:NZ	1:A:85:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ARG:NH2	4:A:1000:PPR:O3P	2.40	0.55
1:A:704:MET:SD	1:A:743:MET:HG2	2.47	0.55
1:A:112:ASN:O	1:A:116:VAL:HG12	2.06	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:144:VAL:HG12	1:A:145:MET:CE	2.37	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:34:MET:CE	1:A:308:LEU:HD22	2.39	0.53
1:A:262:SER:HB3	1:A:400:PRO:HD3	1.88	0.53
1:A:188:LYS:C	1:A:190:ALA:H	2.11	0.53
1:A:704:MET:SD	1:A:764:SER:HB3	2.49	0.53
1:A:519:GLY:C	1:A:521:PHE:H	2.12	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:34:MET:HE2	1:A:308:LEU:HD22	1.92	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:579:ILE:HD12	1:A:623:LEU:HD13	1.92	0.51
1:A:34:MET:SD	1:A:312:LEU:HD21	2.51	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:322:MET:CE	1:A:333:PHE:HE2	2.24	0.50
1:A:757:ALA:HB3	1:A:822:THR:OG1	2.10	0.50
1:A:312:LEU:CD1	1:A:322:MET:HE2	2.23	0.50
1:A:7:LYS:HB2	1:A:10:GLU:HG3	1.93	0.50
1:A:189:GLU:CG	1:A:189:GLU:O	2.58	0.50
1:A:317:ARG:O	1:A:367:ARG:NH1	2.41	0.50
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:573:MET:HE2	1:A:576:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:423:ARG:HH22	1:A:509:ASP:CG	2.15	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:763:PHE:CD2	1:A:826:LEU:HD21	2.48	0.48
1:A:32:LEU:HD22	1:A:311:LYS:HZ2	1.76	0.48
1:A:711:LYS:HD3	1:A:755:ALA:O	2.14	0.48
1:A:504:LYS:C	1:A:505:ILE:HD12	2.33	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:573:MET:HE1	1:A:576:ARG:HH21	1.79	0.47
1:A:289:GLN:HE21	1:A:293:GLN:CD	2.17	0.47
1:A:575:ILE:O	1:A:579:ILE:HG12	2.15	0.47
1:A:548:ASN:O	1:A:551:LYS:HB3	2.13	0.47
1:A:782:ALA:HA	1:A:785:PHE:CE2	2.49	0.47
1:A:689:ILE:HG21	1:A:732:LYS:HD3	1.96	0.47
1:A:551:LYS:HB2	1:A:551:LYS:HE3	1.64	0.47
1:A:482:THR:HA	1:A:490:PHE:O	2.15	0.47
1:A:667:CYS:SG	1:A:717:VAL:HG21	2.55	0.46
1:A:3:LYS:HD2	1:A:3:LYS:HA	1.65	0.46
1:A:295:GLU:HB2	1:A:302:TYR:CD2	2.50	0.46
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: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:162:GLU:C	1:A:164:GLY:N	2.67	0.46
1:A:37:PRO:HB3	1:A:241:THR:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:VAL:HG23	1:A:740:ILE:CD1	2.45	0.46
1:A:537:ARG:HD3	1:A:851:TYR:CD1	2.51	0.46
1:A:521:PHE:CZ	1:A:525:MET:HG3	2.51	0.46
1:A:572:ILE:O	1:A:576:ARG:CG	2.64	0.45
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:546:THR:HG23	1:A:557:ILE:HD11	1.99	0.45
1:A:122:LYS:HD3	1:A:122:LYS:O	2.17	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:148:PRO:O	1:A:150:SER:N	2.49	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: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:468:VAL:HG22	1:A:503:GLY:HA2	1.99	0.45
1:A:82:ASP:OD2	1:A:83:THR:N	2.50	0.45
1:A:557:ILE:HD12	1:A:557:ILE:N	2.32	0.45
1:A:271:GLU:HA	1:A:289:GLN:O	2.17	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: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:244:PHE:HB3	1:A:246:ASN:OD1	2.18	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:518:SER:C	1:A:519:GLY:O	2.50	0.44
1:A:677:ALA:O	1:A:678:LYS:C	2.55	0.44
1:A:424:VAL:CG1	1:A:425:ILE:N	2.80	0.44
1:A:144:VAL:HG12	1:A:145:MET:HE2	2.00	0.44
1:A:688:ALA:O	1:A:692:LYS:HB2	2.17	0.44
1:A:574:LYS:N	1:A:574:LYS:HD2	2.33	0.43
1:A:80:PHE:CE2	1:A:200:PRO:HB2	2.53	0.43
1:A:61:ILE:O	1:A:65:ILE:HG12	2.18	0.43
1:A:436:ILE:CG2	1:A:437:GLU:N	2.81	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:518:SER:O	1:A:521:PHE:CB	2.58	0.43
1:A:230:PRO:HD2	1:A:233:TRP:CE2	2.53	0.43
1:A:830:ILE:HB	1:A:849:LEU:HD21	2.01	0.43
1:A:707:LEU:CD2	1:A:746:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	1:A:209:LYS:HG2	2.01	0.43
1:A:121:LYS:HA	1:A:121:LYS:HD3	1.56	0.43
1:A:59:GLN:CD	1:A:59:GLN:H	2.22	0.43
1:A:499:ASP:OD2	1:A:501:SER:HB2	2.19	0.43
1:A:398:ALA:HB1	1:A:457:ALA:CB	2.49	0.43
1:A:579:ILE:CD1	1:A:623:LEU:HD13	2.49	0.43
1:A:757:ALA:HB3	1:A:822:THR:HG1	1.84	0.43
1:A:808:VAL:O	1:A:808:VAL:HG12	2.19	0.43
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.66	0.43
1:A:42:VAL:HG21	1:A:65:ILE:HD12	2.01	0.42
1:A:689:ILE:HD13	1:A:736:MET:HE3	2.01	0.42
1:A:188:LYS:HG3	1:A:194:GLU:O	2.20	0.42
1:A:685:MET:O	1:A:689:ILE:HG12	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:85:ASP:OD1	1:A:122:LYS:HG3	2.19	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:353:LEU:HA	1:A:353:LEU:HD23	1.82	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:99:MET:HG2	1:A:223:TYR:CE1	2.55	0.41
1:A:148:PRO:O	1:A:149:LYS:C	2.57	0.41
1:A:93:SER:HB3	1:A:211:VAL:HG13	2.02	0.41
1:A:243:VAL:HG11	1:A:332:TYR:CG	2.55	0.41
1:A:7:LYS:HE2	1:A:71:TRP:CD1	2.55	0.41
1:A:765:PHE:CZ	1:A:816:VAL:HG23	2.55	0.41
1:A:284:GLY:HA2	1:A:288:PRO:HD3	2.02	0.41
1:A:514:GLU:HG2	1:A:515:ALA:N	2.35	0.41
1:A:667:CYS:O	1:A:671:VAL:HG23	2.20	0.41
1:A:563:GLU:CG	1:A:621:PRO:HD3	2.51	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:393:GLY:HA3	1:A:485:LEU:HD21	2.03	0.41
1:A:419:GLU:C	1:A:421:GLY:H	2.24	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:557:ILE:O	1:A:557:ILE:HG22	2.19	0.41
1:A:763:PHE:CE2	1:A:826:LEU:HD21	2.55	0.41
1:A:350:ALA:O	1:A:354:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PRO:C	1:A:150:SER:N	2.72	0.41
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.84	0.41
1:A:674:PRO:O	1:A:678:LYS:HG3	2.21	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:399:SER:O	1:A:500:GLY:HA3	2.21	0.40
1:A:689:ILE:HD13	1:A:736:MET:SD	2.61	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:144:VAL:HG12	1:A:145:MET:HE1	2.03	0.40
1:A:3:LYS:HE2	1:A:5:VAL:O	2.22	0.40
1:A:460:ALA:O	1:A:461:ARG:C	2.58	0.40
1:A:277:GLN:O	1:A:278:GLY:C	2.60	0.40
1:A:519:GLY:C	1:A:521:PHE:N	2.75	0.40
1:A:859:VAL:N	1:A:860:PRO:CD	2.84	0.40
1:A:429:LEU:HD11	1:A:449:ARG:HD3	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	870/873 (100%)	820 (94%)	46 (5%)	4 (0%)	34 35

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%)	681 (96%)	32 (4%)	34	41

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	24	CYS
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	157	ASP
1	A	169	THR
1	A	213	ARG
1	A	216	ASP
1	A	268	ILE
1	A	279	GLU
1	A	300	ASP
1	A	322	MET
1	A	458	VAL
1	A	473	GLU
1	A	488	HIS
1	A	505	ILE
1	A	513	GLN
1	A	517	VAL
1	A	520	SER
1	A	576	ARG
1	A	578	MET
1	A	636	GLU
1	A	698	ASP
1	A	743	MET
1	A	747	PRO
1	A	780	ASP

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Mol	Chain	Res	Type
1	A	786	LEU
1	A	830	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	62	GLN
1	A	64	GLN
1	A	138	GLN
1	A	192	ASN
1	A	217	ASN
1	A	440	HIS
1	A	513	GLN
1	A	624	HIS
1	A	727	GLN
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 carbohydrates 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$
4	PPR	A	1000	2	6,9,9	6.45	6 (100%)	7,13,13	1.57	1 (14%)
3	SO4	A	1002	-	4,4,4	0.54	0	6,6,6	0.38	0
3	SO4	A	1003	-	4,4,4	2.98	2 (50%)	6,6,6	1.55	1 (16%)
3	SO4	A	1004	-	4,4,4	0.45	0	6,6,6	0.24	0
3	SO4	A	1005	-	4,4,4	0.60	0	6,6,6	0.53	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	-	0/5/9/9	0/0/0/0
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1000	PPR	C3-C2	-7.51	1.36	1.51
3	A	1003	SO4	O2-S	-4.16	1.32	1.47
3	A	1003	SO4	O4-S	-4.03	1.32	1.47
4	A	1000	PPR	P-O2P	-3.76	1.45	1.54
4	A	1000	PPR	P-O3P	-2.86	1.47	1.54
4	A	1000	PPR	P-O1P	2.59	1.56	1.50
4	A	1000	PPR	O2-C2	5.56	1.32	1.22
4	A	1000	PPR	P-C3	11.55	1.96	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1000	PPR	O3P-P-O2P	2.51	115.49	108.13
3	A	1003	SO4	O4-S-O3	3.42	122.88	108.98

There are no chirality outliers.

There are no torsion outliers.

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, 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	872/873 (99%)	0.36	33 (3%) 44 43	3, 26, 61, 85	10 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ASN	6.7
1	A	165	VAL	5.1
1	A	164	GLY	4.2
1	A	518	SER	4.0
1	A	388	ALA	4.0
1	A	167	PHE	3.9
1	A	163	LYS	3.6
1	A	162	GLU	3.4
1	A	519	GLY	3.2
1	A	166	HIS	3.1
1	A	490	PHE	3.1
1	A	516	SER	3.0
1	A	191	MET	3.0
1	A	488	HIS	2.8
1	A	158	ALA	2.7
1	A	52	ASN	2.6
1	A	486	GLY	2.6
1	A	640	ASN	2.5
1	A	189	GLU	2.4
1	A	631	GLU	2.4
1	A	510	ILE	2.3
1	A	278	GLY	2.3
1	A	661	MET	2.2
1	A	485	LEU	2.2
1	A	477	ASN	2.2
1	A	195	GLU	2.2
1	A	193	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.1
1	A	520	SER	2.1
1	A	708	VAL	2.1
1	A	630	THR	2.0
1	A	386	LEU	2.0
1	A	161	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PPR	A	1000	10/10	0.81	0.22	1.66	3,18,21,23	0
3	SO4	A	1002	5/5	0.98	0.15	-0.34	18,23,25,31	0
3	SO4	A	1005	5/5	0.94	0.14	-0.73	20,39,49,53	0
2	MG	A	1001	1/1	0.84	0.12	-4.44	7,7,7,7	0
3	SO4	A	1004	5/5	0.85	0.17	-	36,50,54,60	0
3	SO4	A	1003	5/5	0.90	0.21	-	2,16,19,20	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.