



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:39 PM UTC

PDB ID : 1VBH / pdb_00001vbh
Title : Pyruvate Phosphate Dikinase with bound Mg-PEP from Maize
Authors : Nakanishi, T.; Nakatsu, T.; Matsuoka, M.; Sakata, K.; Kato, H.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-02-26
Resolution : 2.30 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

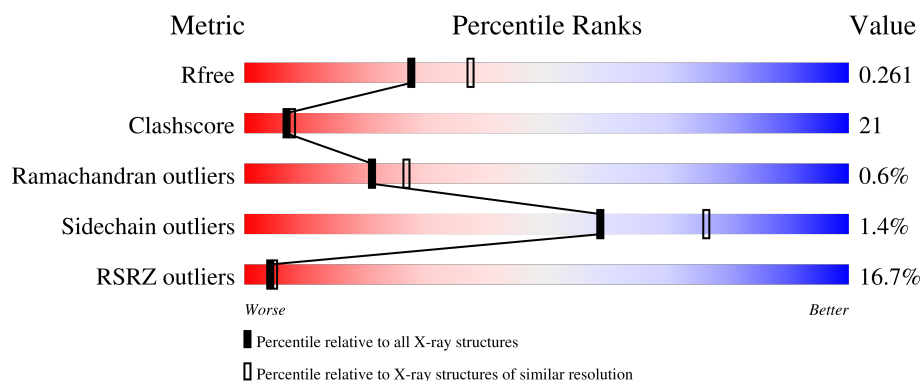
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	876	16% 67% 31% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6665 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,orthophosphate dikinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	862	6455	4083	1122	1204	46	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	819	PHE	LEU	SEE REMARK 999	UNP P11155

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

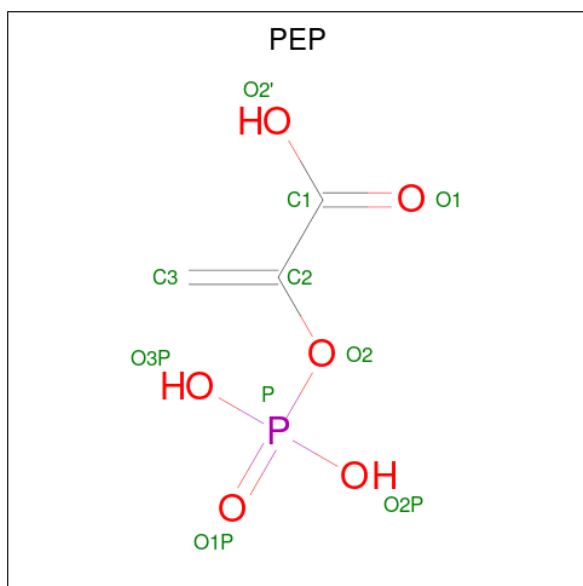
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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		

- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



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

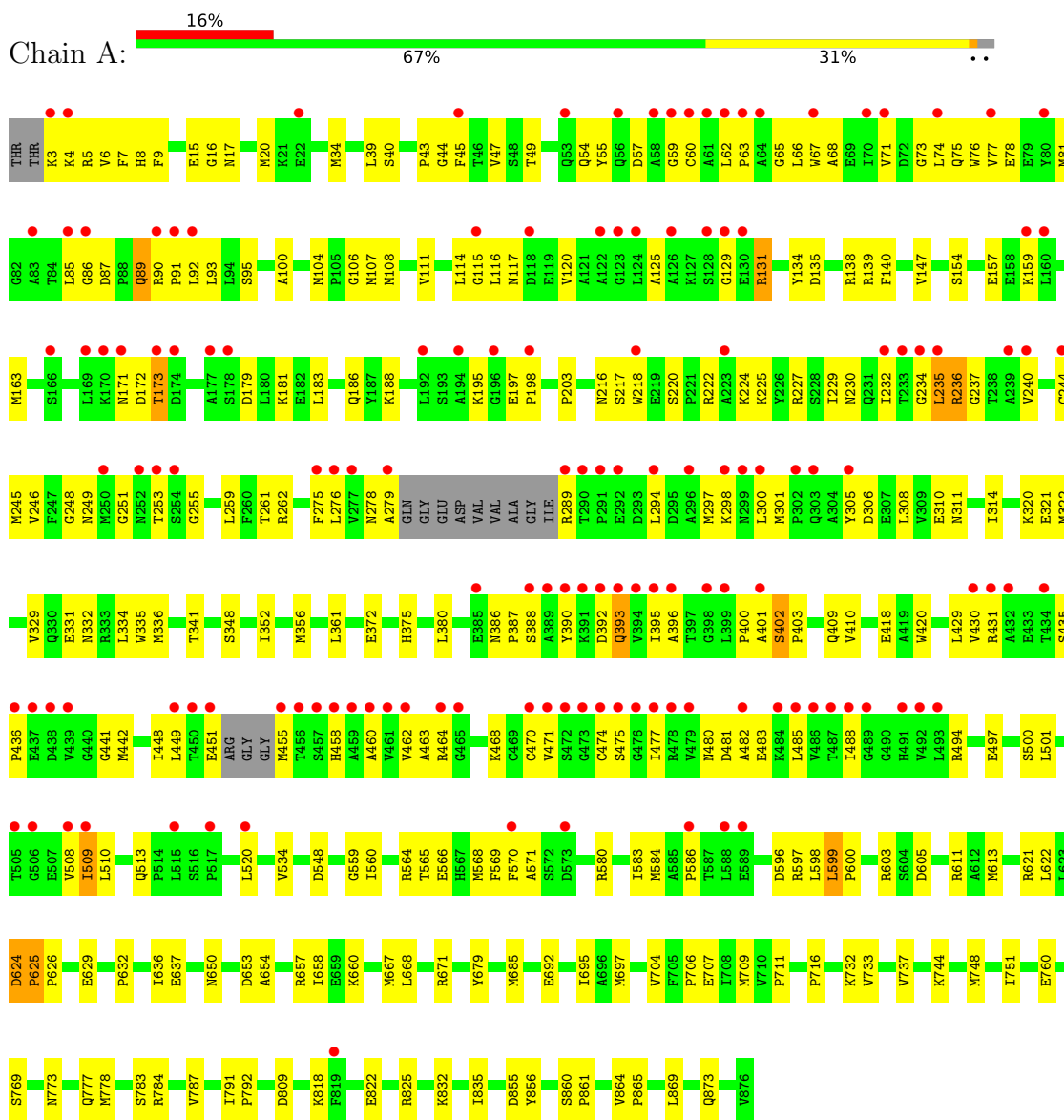
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		

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: pyruvate,orthophosphate dikinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.34Å 100.51Å 108.16Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	45.63 – 2.30 45.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.63-2.30) 98.1 (45.63-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.259 0.231 , 0.261	Depositor DCC
R_{free} test set	2528 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6665	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: PEP, 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	0.53	0/6577	0.94	11/8913 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	VAL	N-CA-C	6.59	117.38	110.72
1	A	679	TYR	CA-C-N	6.22	126.42	119.32
1	A	679	TYR	C-N-CA	6.22	126.42	119.32
1	A	294	LEU	N-CA-C	6.11	117.61	111.07
1	A	625	PRO	N-CA-C	5.88	116.87	110.58
1	A	625	PRO	CB-CA-C	-5.78	105.74	111.17
1	A	90	ARG	CA-C-N	5.43	125.36	119.76
1	A	90	ARG	C-N-CA	5.43	125.36	119.76
1	A	402	SER	CA-C-N	5.43	125.43	119.89
1	A	402	SER	C-N-CA	5.43	125.43	119.89
1	A	570	PHE	N-CA-C	-5.27	107.15	113.21

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	6455	0	6308	270	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	10	0	2	2	0
5	A	194	0	0	8	0
All	All	6665	0	6310	270	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 (270) 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:131:ARG:H	1:A:131:ARG:HD3	1.21	1.02
1:A:509:ILE:HD12	1:A:509:ILE:H	1.25	1.00
1:A:777:GLN:NE2	1:A:784:ARG:H	1.62	0.97
1:A:777:GLN:HE21	1:A:784:ARG:H	1.04	0.93
1:A:74:LEU:HD12	1:A:75:GLN:N	1.88	0.88
1:A:429:LEU:HD21	1:A:431:ARG:HG3	1.58	0.84
1:A:387:PRO:HA	1:A:390:TYR:CE2	2.13	0.84
1:A:596:ASP:O	1:A:600:PRO:HD3	1.77	0.84
1:A:787:VAL:HG22	1:A:791:ILE:HG12	1.60	0.82
1:A:668:LEU:HD21	1:A:778[B]:MET:HE1	1.60	0.82
1:A:477:ILE:CG1	1:A:488:ILE:HG12	2.09	0.81
1:A:253:THR:HG22	1:A:332:ASN:N	1.98	0.79
1:A:195:LYS:HA	1:A:195:LYS:HE2	1.63	0.78
1:A:81:MET:HE2	1:A:244[B]:CYS:SG	2.23	0.78
1:A:396:ALA:HB3	1:A:508:VAL:CG2	2.15	0.76
1:A:396:ALA:HB3	1:A:508:VAL:HG21	1.66	0.76
1:A:668:LEU:HD21	1:A:778[B]:MET:CE	2.16	0.76
1:A:40:SER:H	1:A:311:ASN:HD21	1.31	0.75
1:A:401:ALA:HB1	1:A:460:ALA:CB	2.17	0.75
1:A:372:GLU:H	1:A:375:HIS:HD2	1.33	0.74
1:A:668:LEU:HD21	1:A:778[B]:MET:SD	2.28	0.74
1:A:356:MET:HE3	1:A:361:LEU:HD23	1.70	0.73
1:A:566:GLU:HG3	1:A:625:PRO:HG3	1.71	0.72
1:A:67:TRP:O	1:A:71:VAL:HG23	1.90	0.71
1:A:249:ASN:HA	1:A:278:ASN:ND2	2.06	0.71
1:A:668:LEU:CD2	1:A:778[B]:MET:HE1	2.20	0.71
1:A:5:ARG:NH2	1:A:63:PRO:HB2	2.06	0.70
1:A:455:MET:HE3	1:A:464:ARG:NH2	2.06	0.70
1:A:777:GLN:HE21	1:A:784:ARG:N	1.85	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD22	1:A:279:ALA:HB3	1.72	0.69
1:A:259:LEU:HD12	1:A:259:LEU:C	2.18	0.69
1:A:509:ILE:HD12	1:A:509:ILE:N	2.04	0.69
1:A:559:GLY:HA2	1:A:613:MET:CE	2.23	0.69
1:A:251:GLY:C	5:A:3095:HOH:O	2.35	0.68
1:A:474:CYS:O	1:A:477:ILE:HG22	1.93	0.68
1:A:431:ARG:HG2	1:A:431:ARG:HH11	1.58	0.68
1:A:621:ARG:HH11	1:A:748:MET:HE2	1.58	0.68
1:A:356:MET:HE3	1:A:361:LEU:CD2	2.22	0.68
1:A:626:PRO:HD2	1:A:629:GLU:OE2	1.94	0.68
1:A:321:GLU:CG	1:A:341:THR:HG23	2.24	0.67
1:A:787:VAL:HG22	1:A:791:ILE:CG1	2.25	0.67
1:A:188:LYS:HB3	5:A:3177:HOH:O	1.94	0.67
1:A:87:ASP:OD1	1:A:89:GLN:HG3	1.93	0.67
1:A:520:LEU:O	1:A:520:LEU:HD23	1.94	0.67
1:A:297:MET:HE2	1:A:305:TYR:HA	1.77	0.67
1:A:154:SER:HA	1:A:157:GLU:HG2	1.75	0.66
1:A:3:LYS:HZ1	1:A:8:HIS:CE1	2.13	0.66
1:A:401:ALA:HB1	1:A:460:ALA:HB2	1.78	0.66
1:A:509:ILE:H	1:A:509:ILE:CD1	2.00	0.66
1:A:380:LEU:HD13	1:A:865:PRO:HG2	1.77	0.66
1:A:17:ASN:H	1:A:20:MET:HE3	1.58	0.66
1:A:458:HIS:O	1:A:462:VAL:HG23	1.96	0.65
1:A:372:GLU:H	1:A:375:HIS:CD2	2.13	0.65
1:A:125:ALA:HA	1:A:129:GLY:O	1.96	0.65
1:A:249:ASN:HA	1:A:278:ASN:HD22	1.60	0.65
1:A:5:ARG:HH22	1:A:63:PRO:HB2	1.61	0.64
1:A:390:TYR:HA	1:A:393:GLN:NE2	2.12	0.64
1:A:624:ASP:O	1:A:671[A]:ARG:HB2	1.96	0.64
1:A:310:GLU:O	1:A:314:ILE:HG12	1.98	0.64
1:A:596:ASP:O	1:A:600:PRO:CD	2.44	0.64
1:A:17:ASN:N	1:A:20:MET:HE3	2.12	0.64
1:A:429:LEU:C	1:A:429:LEU:HD23	2.23	0.64
1:A:89:GLN:C	1:A:91:PRO:HD3	2.23	0.63
1:A:695:ILE:HG21	1:A:737:VAL:HG21	1.80	0.63
1:A:107:MET:HE2	1:A:218:TRP:CE3	2.33	0.63
1:A:751:ILE:HD13	1:A:778[A]:MET:SD	2.39	0.62
1:A:275:PHE:CE2	1:A:301:MET:HE1	2.34	0.62
1:A:508:VAL:HG23	1:A:508:VAL:O	1.99	0.61
1:A:603:ARG:NH1	1:A:692:GLU:OE1	2.30	0.61
1:A:154:SER:HA	1:A:157:GLU:CD	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ARG:O	1:A:497:GLU:HG3	2.02	0.59
1:A:597:ARG:O	1:A:600:PRO:HD2	2.01	0.59
1:A:321:GLU:HG2	1:A:341:THR:HG23	1.83	0.59
1:A:16:GLY:HA2	1:A:20:MET:HE1	1.85	0.59
1:A:485:LEU:HB3	1:A:494:ARG:HG2	1.84	0.59
1:A:624:ASP:O	1:A:671[B]:ARG:HB2	2.01	0.59
1:A:429:LEU:CD2	1:A:431:ARG:HG3	2.32	0.58
1:A:107:MET:HE2	1:A:218:TRP:HE3	1.67	0.58
1:A:74:LEU:O	1:A:78:GLU:HG3	2.03	0.58
1:A:566:GLU:CD	1:A:625:PRO:HD3	2.29	0.58
1:A:667[B]:MET:HE2	1:A:777:GLN:NE2	2.19	0.58
1:A:429:LEU:HD23	1:A:430:VAL:N	2.18	0.57
1:A:569:PHE:C	1:A:571:ALA:H	2.12	0.57
1:A:380:LEU:CD1	1:A:865:PRO:HG2	2.33	0.57
1:A:455:MET:HE3	1:A:464:ARG:HH21	1.68	0.57
1:A:163:MET:HE1	1:A:179:ASP:O	2.05	0.57
1:A:733:VAL:O	1:A:737:VAL:HG12	2.05	0.57
1:A:387:PRO:HA	1:A:390:TYR:CZ	2.40	0.57
1:A:599:LEU:HB3	1:A:600:PRO:HD3	1.86	0.57
1:A:654:ALA:O	1:A:658:ILE:HG13	2.04	0.57
1:A:154:SER:HA	1:A:157:GLU:CG	2.35	0.56
1:A:5:ARG:CZ	1:A:54:GLN:HE22	2.19	0.56
1:A:73:GLY:O	1:A:77:VAL:HG23	2.06	0.56
1:A:251:GLY:CA	5:A:3095:HOH:O	2.54	0.56
1:A:667[B]:MET:HE2	1:A:777:GLN:CD	2.29	0.56
1:A:55:TYR:O	1:A:60:CYS:HA	2.06	0.55
1:A:62:LEU:HD23	1:A:63:PRO:O	2.06	0.55
1:A:667[B]:MET:HE1	1:A:783:SER:HA	1.87	0.55
1:A:455:MET:O	1:A:464:ARG:NH2	2.39	0.55
1:A:17:ASN:ND2	1:A:20:MET:HE2	2.22	0.55
1:A:78:GLU:HG2	1:A:92:LEU:CD2	2.37	0.55
1:A:235:LEU:O	1:A:236:ARG:HB3	2.07	0.55
1:A:43:PRO:HG3	1:A:81:MET:HG2	1.89	0.55
1:A:172:ASP:O	1:A:173:THR:HB	2.08	0.54
1:A:235:LEU:O	1:A:236:ARG:CB	2.55	0.54
1:A:481:ASP:O	1:A:482:ALA:C	2.50	0.54
1:A:100:ALA:HB2	1:A:107:MET:HE1	1.89	0.54
1:A:864:VAL:HB	1:A:865:PRO:HD3	1.89	0.54
1:A:435:SER:HB2	1:A:436:PRO:HD2	1.88	0.54
1:A:480:ASN:O	1:A:483:GLU:O	2.24	0.54
1:A:598:LEU:HB2	1:A:685:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HD3	1:A:235:LEU:HD12	1.88	0.54
1:A:611[A]:ARG:NH1	1:A:697:MET:SD	2.80	0.54
1:A:197:GLU:HB2	1:A:198:PRO:HD2	1.88	0.54
1:A:108:MET:HE3	1:A:111:VAL:HG23	1.90	0.54
1:A:71:VAL:O	1:A:74:LEU:HG	2.07	0.53
1:A:513:GLN:HE21	1:A:513:GLN:HA	1.73	0.53
1:A:636:ILE:HG23	1:A:637:GLU:N	2.24	0.53
1:A:568:MET:CE	1:A:605:ASP:HB3	2.39	0.53
1:A:85:LEU:HG	1:A:203:PRO:HB3	1.91	0.53
1:A:400:PRO:HG2	1:A:455:MET:SD	2.48	0.53
1:A:485:LEU:HD12	1:A:485:LEU:C	2.34	0.53
1:A:16:GLY:HA2	1:A:20:MET:CE	2.38	0.52
1:A:159:LYS:HD3	1:A:186:GLN:HB3	1.91	0.52
1:A:621:ARG:NH1	1:A:748:MET:HE2	2.25	0.52
1:A:8:HIS:CE1	1:A:76:TRP:CZ2	2.98	0.52
1:A:225:LYS:O	1:A:229:ILE:HG13	2.09	0.52
1:A:401:ALA:HB3	1:A:470:CYS:O	2.10	0.52
1:A:509:ILE:HG22	1:A:510:LEU:N	2.24	0.52
1:A:227:ARG:HA	1:A:232:ILE:HD12	1.92	0.52
1:A:650:ASN:ND2	1:A:653:ASP:H	2.08	0.52
1:A:560:ILE:HG13	1:A:613:MET:HE2	1.92	0.52
1:A:131:ARG:HD3	1:A:131:ARG:N	2.06	0.51
1:A:138:ARG:HD2	1:A:183:LEU:HD23	1.90	0.51
1:A:278:ASN:HD22	1:A:278:ASN:C	2.18	0.51
1:A:78:GLU:HG2	1:A:92:LEU:HD22	1.91	0.51
1:A:395:ILE:O	1:A:396:ALA:HB2	2.10	0.51
1:A:246:VAL:HG11	1:A:335:TRP:CD1	2.46	0.51
1:A:500:SER:HB2	1:A:509:ILE:HB	1.93	0.51
1:A:869:LEU:O	1:A:873:GLN:HG3	2.11	0.51
1:A:777:GLN:NE2	1:A:784:ARG:N	2.46	0.51
1:A:732:LYS:NZ	5:A:3161:HOH:O	2.41	0.50
1:A:449:LEU:HD12	1:A:471:VAL:O	2.11	0.50
1:A:171:ASN:O	1:A:173:THR:HG22	2.11	0.50
1:A:856:TYR:CD1	1:A:856:TYR:C	2.90	0.49
1:A:134:TYR:CE2	1:A:181:LYS:HE2	2.48	0.49
1:A:230:ASN:HB2	1:A:232:ILE:CG1	2.42	0.49
1:A:320:LYS:C	1:A:356:MET:HE1	2.38	0.49
1:A:860:SER:HB2	1:A:861:PRO:HD2	1.95	0.49
1:A:580:ARG:CZ	1:A:632:PRO:HG3	2.42	0.49
1:A:773:ASN:HB2	4:A:3000:PEP:C1	2.42	0.49
1:A:117:ASN:OD1	1:A:120:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HG22	1:A:235:LEU:HD21	1.94	0.49
1:A:597:ARG:C	1:A:600:PRO:HD2	2.38	0.49
1:A:818:LYS:O	1:A:822:GLU:HG3	2.12	0.49
1:A:513:GLN:HA	1:A:513:GLN:NE2	2.28	0.48
1:A:564:ARG:HH21	4:A:3000:PEP:P	2.36	0.48
1:A:251:GLY:HA3	5:A:3095:HOH:O	2.13	0.48
1:A:386:ASN:OD1	1:A:388:SER:HB3	2.12	0.48
1:A:566:GLU:CB	1:A:625:PRO:CG	2.92	0.48
1:A:463:ALA:HB1	1:A:468:LYS:O	2.14	0.48
1:A:611[A]:ARG:NH1	1:A:611[A]:ARG:HB2	2.29	0.48
1:A:114:LEU:C	1:A:114:LEU:HD23	2.39	0.48
1:A:707:GLU:HG2	1:A:744:LYS:HB2	1.96	0.48
1:A:107:MET:CE	1:A:218:TRP:CZ3	2.97	0.47
1:A:431:ARG:HG2	1:A:431:ARG:NH1	2.28	0.47
1:A:475:SER:C	1:A:477:ILE:H	2.21	0.47
1:A:49:THR:OG1	1:A:236:ARG:HD3	2.13	0.47
1:A:188:LYS:O	5:A:3177:HOH:O	2.20	0.47
1:A:298:LYS:C	1:A:300:LEU:H	2.22	0.47
1:A:400:PRO:C	1:A:455:MET:SD	2.97	0.47
1:A:509:ILE:HG22	1:A:510:LEU:H	1.80	0.47
1:A:451:GLU:CB	1:A:477:ILE:CG2	2.92	0.47
1:A:131:ARG:H	1:A:131:ARG:CD	2.04	0.47
1:A:154:SER:O	1:A:157:GLU:HG2	2.15	0.47
1:A:261:THR:OG1	1:A:322:MET:HG2	2.15	0.47
1:A:7:PHE:O	1:A:45:PHE:HA	2.15	0.47
1:A:135:ASP:OD1	1:A:138:ARG:NH1	2.48	0.46
1:A:138:ARG:CG	1:A:139:ARG:N	2.78	0.46
1:A:297:MET:HE2	1:A:305:TYR:CA	2.44	0.46
1:A:3:LYS:HB3	1:A:6:VAL:O	2.15	0.46
1:A:114:LEU:HA	1:A:140:PHE:CE1	2.50	0.46
1:A:74:LEU:HD12	1:A:74:LEU:C	2.39	0.46
1:A:62:LEU:HD23	1:A:62:LEU:C	2.41	0.46
1:A:321:GLU:HG3	1:A:341:THR:HG23	1.96	0.46
1:A:275:PHE:HE2	1:A:301:MET:HE1	1.80	0.46
1:A:3:LYS:HD2	1:A:15:GLU:CB	2.46	0.46
1:A:95:SER:HB3	1:A:245:MET:SD	2.56	0.46
1:A:429:LEU:C	1:A:429:LEU:CD2	2.89	0.46
1:A:401:ALA:CB	1:A:460:ALA:HB2	2.46	0.45
1:A:791:ILE:HB	1:A:792:PRO:HD3	1.97	0.45
1:A:47:VAL:HB	1:A:240:VAL:HB	1.99	0.45
1:A:220:SER:O	1:A:224:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:VAL:HG12	1:A:706:PRO:HD3	1.98	0.45
1:A:5:ARG:NH2	1:A:66:LEU:HB2	2.31	0.45
1:A:660:LYS:HE3	1:A:660:LYS:HB2	1.80	0.45
1:A:71:VAL:HA	1:A:74:LEU:HG	1.98	0.45
1:A:255:GLY:HA3	1:A:275:PHE:CZ	2.52	0.45
1:A:650:ASN:HD21	1:A:653:ASP:H	1.64	0.45
1:A:108:MET:HG3	1:A:147:VAL:CG1	2.46	0.44
1:A:548:ASP:OD2	5:A:3150:HOH:O	2.21	0.44
1:A:667[B]:MET:CE	1:A:783:SER:HA	2.48	0.44
1:A:3:LYS:HZ1	1:A:8:HIS:CD2	2.34	0.44
1:A:3:LYS:NZ	1:A:8:HIS:CD2	2.85	0.44
1:A:348:SER:O	1:A:352:ILE:HG13	2.17	0.44
1:A:393:GLN:HE21	1:A:393:GLN:N	2.15	0.44
1:A:57:ASP:C	1:A:59:GLY:H	2.25	0.44
1:A:85:LEU:HG	1:A:203:PRO:CB	2.48	0.44
1:A:709:MET:SD	1:A:769:SER:HB3	2.57	0.44
1:A:716:PRO:HG3	1:A:760:GLU:HB3	2.00	0.44
1:A:234:GLY:O	1:A:235:LEU:C	2.60	0.44
1:A:259:LEU:C	1:A:259:LEU:CD1	2.87	0.44
1:A:253:THR:HG22	1:A:331:GLU:C	2.43	0.44
1:A:566:GLU:CG	1:A:625:PRO:HG3	2.45	0.44
1:A:106:GLY:N	1:A:222:ARG:HD3	2.33	0.44
1:A:259:LEU:HD12	1:A:259:LEU:O	2.18	0.43
1:A:409:GLN:NE2	1:A:420:TRP:HE1	2.16	0.43
1:A:583:ILE:O	1:A:583:ILE:HG22	2.17	0.43
1:A:624:ASP:H	1:A:625:PRO:HD2	1.83	0.43
1:A:624:ASP:H	1:A:625:PRO:CD	2.31	0.43
1:A:832:LYS:HE3	5:A:3036:HOH:O	2.17	0.43
1:A:108:MET:H	1:A:217:SER:CB	2.31	0.43
1:A:329:VAL:O	1:A:329:VAL:HG13	2.18	0.43
1:A:773:ASN:O	1:A:777:GLN:HG3	2.19	0.43
1:A:34:MET:O	1:A:39:LEU:HB2	2.18	0.43
1:A:276:LEU:HD21	1:A:289:ARG:HD3	2.01	0.43
1:A:402:SER:HA	1:A:403:PRO:HD2	1.88	0.43
1:A:395:ILE:HG12	1:A:508:VAL:O	2.18	0.43
1:A:501:LEU:CD2	1:A:508:VAL:HG12	2.49	0.43
1:A:114:LEU:HD23	1:A:115:GLY:N	2.33	0.43
1:A:311:ASN:HB3	1:A:336:MET:HE3	2.01	0.43
1:A:622:LEU:O	1:A:711:PRO:HG3	2.19	0.43
1:A:43:PRO:CG	1:A:81:MET:HG2	2.48	0.42
1:A:253:THR:HG22	1:A:253:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:GLY:HA2	1:A:613:MET:HE3	1.98	0.42
1:A:449:LEU:HB2	1:A:501:LEU:HD11	2.01	0.42
1:A:825:ARG:NH2	1:A:855:ASP:OD2	2.47	0.42
1:A:442:MET:HE2	1:A:448:ILE:HD13	2.02	0.42
1:A:8:HIS:HA	1:A:45:PHE:HA	2.01	0.42
1:A:565:THR:HA	1:A:568:MET:HG3	2.02	0.42
1:A:569:PHE:C	1:A:571:ALA:N	2.77	0.42
1:A:4:LYS:O	1:A:4:LYS:HG2	2.20	0.42
1:A:108:MET:HG3	1:A:147:VAL:HG12	2.02	0.42
1:A:410:VAL:HG23	1:A:497:GLU:O	2.19	0.42
1:A:418:GLU:HG3	1:A:441:GLY:HA2	2.01	0.42
1:A:668:LEU:CD2	1:A:778[B]:MET:CE	2.88	0.42
1:A:9:PHE:N	1:A:44:GLY:O	2.50	0.42
1:A:249:ASN:CA	1:A:278:ASN:ND2	2.81	0.42
1:A:390:TYR:CD1	1:A:390:TYR:C	2.97	0.42
1:A:138:ARG:HG2	1:A:139:ARG:N	2.35	0.41
1:A:227:ARG:HG3	1:A:232:ILE:HB	2.01	0.41
1:A:559:GLY:CA	1:A:613:MET:CE	2.96	0.41
1:A:65:GLY:O	1:A:68:ALA:HB3	2.20	0.41
1:A:248:GLY:O	1:A:278:ASN:HA	2.20	0.41
1:A:451:GLU:CB	1:A:477:ILE:HG23	2.50	0.41
1:A:104:MET:CE	1:A:227:ARG:HH21	2.33	0.41
1:A:261:THR:O	1:A:262:ARG:HG2	2.19	0.41
1:A:86:GLY:HA3	1:A:203:PRO:HG2	2.02	0.41
1:A:93:LEU:HD21	1:A:116:LEU:HD13	2.03	0.41
1:A:107:MET:CE	1:A:218:TRP:HZ3	2.34	0.41
1:A:253:THR:HG23	1:A:332:ASN:ND2	2.35	0.41
1:A:584:MET:SD	1:A:657:ARG:HG2	2.60	0.41
1:A:55:TYR:HE2	1:A:216:ASN:ND2	2.19	0.41
1:A:218:TRP:CE2	1:A:237:GLY:HA2	2.56	0.40
1:A:509:ILE:HG21	1:A:513:GLN:HG3	2.02	0.40
1:A:611[A]:ARG:HB2	1:A:611[A]:ARG:HH11	1.86	0.40
1:A:308:LEU:N	1:A:334:LEU:HD22	2.36	0.40
1:A:395:ILE:HD13	1:A:510:LEU:HD13	2.04	0.40
1:A:401:ALA:HB1	1:A:460:ALA:CA	2.51	0.40
1:A:667[A]:MET:O	1:A:668:LEU:HD23	2.22	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	864/876 (99%)	809 (94%)	50 (6%)	5 (1%)	21	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR
1	A	235	LEU
1	A	236	ARG
1	A	586	PRO
1	A	624	ASP

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	653/707 (92%)	644 (99%)	9 (1%)	59	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	131	ARG
1	A	306	ASP
1	A	392	ASP
1	A	393	GLN
1	A	509	ILE

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Mol	Chain	Res	Type
1	A	599	LEU
1	A	809	ASP
1	A	835	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	146	ASN
1	A	216	ASN
1	A	252	ASN
1	A	278	ASN
1	A	311	ASN
1	A	318	HIS
1	A	330	GLN
1	A	332	ASN
1	A	338	GLN
1	A	375	HIS
1	A	393	GLN
1	A	409	GLN
1	A	602	GLN
1	A	650	ASN
1	A	651	GLN
1	A	722	GLN
1	A	764	GLN
1	A	777	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	PEP	A	3000	2	9,9,9	3.70	4 (44%)	11,13,13	2.71	3 (27%)
3	SO4	A	3001	-	4,4,4	0.37	0	6,6,6	0.09	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	PEP	A	3000	2	-	0/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	PEP	C2-C1	8.53	1.57	1.49
4	A	3000	PEP	O2'-C1	-4.96	1.17	1.30
4	A	3000	PEP	P-O2	3.23	1.65	1.59
4	A	3000	PEP	P-O2P	-2.08	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3000	PEP	O2'-C1-C2	7.49	126.69	113.91
4	A	3000	PEP	O1-C1-C2	-3.78	116.09	121.79
4	A	3000	PEP	O2'-C1-O1	-2.81	117.22	123.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3000	PEP	2	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	862/876 (98%)	0.89	144 (16%) 4 5	9, 51, 81, 94	8 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	5.7
1	A	235	LEU	5.3
1	A	461	VAL	5.1
1	A	476	GLY	4.8
1	A	299	ASN	4.5
1	A	279	ALA	4.3
1	A	171	ASN	4.3
1	A	488	ILE	4.2
1	A	459	ALA	4.1
1	A	296	ALA	4.0
1	A	169	LEU	4.0
1	A	388	SER	4.0
1	A	118	ASP	3.8
1	A	458	HIS	3.9
1	A	91	PRO	3.8
1	A	460	ALA	3.8
1	A	174	ASP	3.8
1	A	432	ALA	3.8
1	A	303	GLN	3.7
1	A	486	VAL	3.7
1	A	177	ALA	3.6
1	A	396	ALA	3.6
1	A	462	VAL	3.6
1	A	472	SER	3.5
1	A	92	LEU	3.5
1	A	508	VAL	3.5
1	A	401	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	455	MET	3.5
1	A	475	SER	3.5
1	A	45	PHE	3.5
1	A	437	GLU	3.5
1	A	56	GLN	3.5
1	A	477	ILE	3.5
1	A	471	VAL	3.4
1	A	61	ALA	3.4
1	A	302	PRO	3.3
1	A	124	LEU	3.3
1	A	160	LEU	3.3
1	A	588	LEU	3.3
1	A	450	THR	3.3
1	A	80	TYR	3.2
1	A	479	VAL	3.2
1	A	233	THR	3.2
1	A	506	GLY	3.2
1	A	399	LEU	3.2
1	A	62	LEU	3.1
1	A	4	LYS	3.1
1	A	439	VAL	3.1
1	A	196	GLY	3.1
1	A	457	SER	3.1
1	A	485	LEU	3.1
1	A	292	GLU	3.0
1	A	115	GLY	3.0
1	A	122	ALA	3.0
1	A	395	ILE	3.0
1	A	67	TRP	3.0
1	A	473	GLY	3.0
1	A	487	THR	3.0
1	A	64	ALA	2.9
1	A	83	ALA	2.9
1	A	276	LEU	2.9
1	A	244[A]	CYS	2.9
1	A	294	LEU	2.9
1	A	128	SER	2.9
1	A	86	GLY	2.9
1	A	819[A]	PHE	2.9
1	A	59	GLY	2.8
1	A	277	VAL	2.8
1	A	60	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	465	GLY	2.8
1	A	586	PRO	2.8
1	A	85	LEU	2.8
1	A	71	VAL	2.8
1	A	290	THR	2.8
1	A	3	LYS	2.8
1	A	464	ARG	2.8
1	A	63	PRO	2.7
1	A	253	THR	2.7
1	A	484	LYS	2.7
1	A	394	VAL	2.7
1	A	482	ALA	2.7
1	A	491	HIS	2.6
1	A	492	VAL	2.6
1	A	170	LYS	2.6
1	A	239	ALA	2.6
1	A	505	THR	2.6
1	A	300	LEU	2.5
1	A	58	ALA	2.5
1	A	194	ALA	2.5
1	A	470	CYS	2.5
1	A	474	CYS	2.5
1	A	489	GLY	2.5
1	A	509	ILE	2.5
1	A	431	ARG	2.5
1	A	130	GLU	2.5
1	A	493	LEU	2.5
1	A	385	GLU	2.4
1	A	70	ILE	2.4
1	A	77	VAL	2.4
1	A	390	TYR	2.4
1	A	298	LYS	2.4
1	A	456	THR	2.4
1	A	275	PHE	2.4
1	A	520	LEU	2.4
1	A	451	GLU	2.4
1	A	291	PRO	2.4
1	A	123	GLY	2.4
1	A	393	GLN	2.4
1	A	438	ASP	2.3
1	A	159	LYS	2.3
1	A	570	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	398	GLY	2.3
1	A	449	LEU	2.3
1	A	436	PRO	2.3
1	A	391	LYS	2.3
1	A	223	ALA	2.3
1	A	434	THR	2.3
1	A	478	ARG	2.2
1	A	53	GLN	2.2
1	A	173	THR	2.2
1	A	234	GLY	2.2
1	A	218	TRP	2.2
1	A	289	ARG	2.2
1	A	178	SER	2.2
1	A	389	ALA	2.2
1	A	192	LEU	2.1
1	A	515	LEU	2.1
1	A	129	GLY	2.1
1	A	90	ARG	2.1
1	A	252	ASN	2.1
1	A	589	GLU	2.1
1	A	126	ALA	2.1
1	A	166	SER	2.1
1	A	250	MET	2.1
1	A	305	TYR	2.1
1	A	240	VAL	2.1
1	A	517	PRO	2.1
1	A	392	ASP	2.1
1	A	22	GLU	2.0
1	A	198	PRO	2.0
1	A	430	VAL	2.0
1	A	254	SER	2.0
1	A	573	ASP	2.0
1	A	232	ILE	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	3001	5/5	0.89	0.09	80,80,81,81	0
2	MG	A	2000	1/1	0.93	0.09	38,38,38,38	0
4	PEP	A	3000	10/10	0.93	0.10	38,42,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.