



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:41 AM UTC

PDB ID : 2AL2 / pdb_00002al2
Title : Crystal Structure Analysis of Enolase Mg Subunit Complex at pH 8.0
Authors : Sims, P.A.; Menefee, A.L.; Larsen, T.M.; Mansoorabadi, S.O.; Reed, G.H.
Deposited on : 2005-08-04
Resolution : 1.85 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

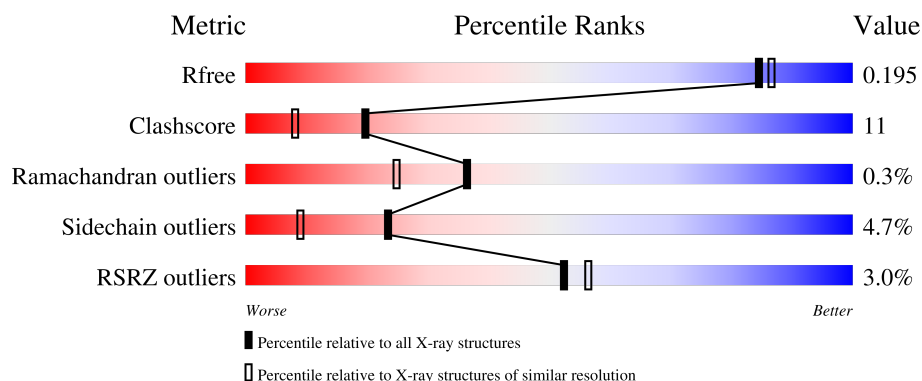
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	436	2% 77% 22% .
2	B	436	4% 71% 25% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7128 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 enolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3288	2076	569	637	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	ALA	LYS	engineered mutation	UNP P00924

- Molecule 2 is a protein called enolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3257	2060	560	631	6			

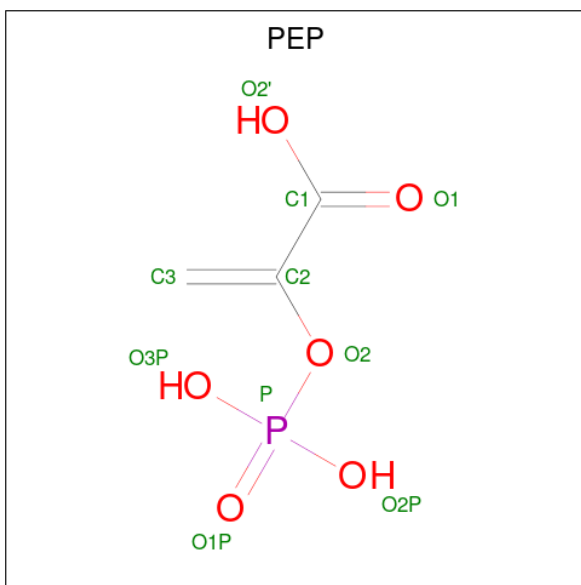
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	80	ASP	ASN	engineered mutation	UNP P00924
B	126	ASP	ASN	engineered mutation	UNP P00924

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

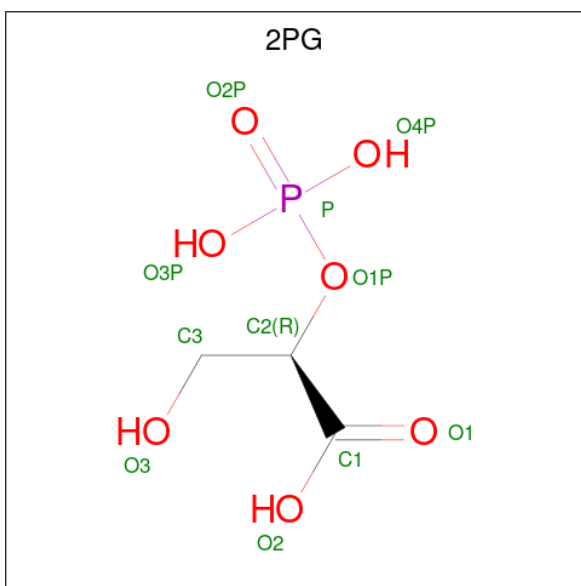
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



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

- Molecule 5 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: $\text{C}_3\text{H}_7\text{O}_7\text{P}$).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	K 1	0	0

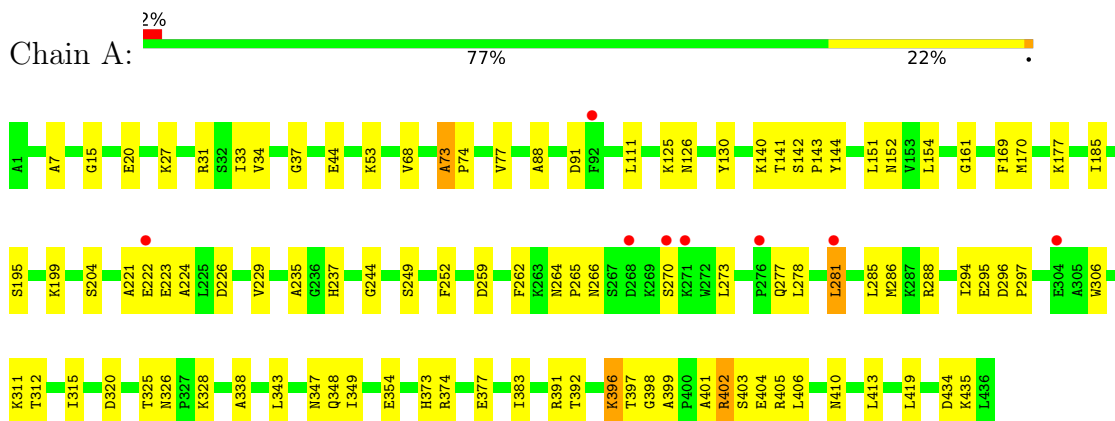
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total 274	O 274	0	0
8	B	261	Total 261	O 261	0	0

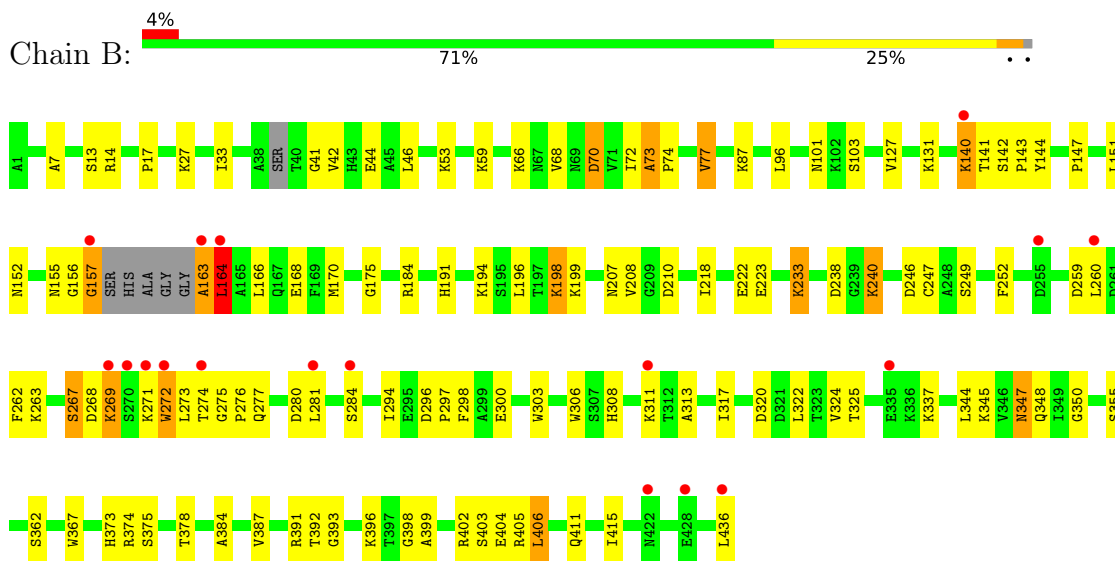
3 Residue-property plots [i](#)

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: enolase 1



- Molecule 2: enolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.70Å 65.60Å 85.90Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	26.00 – 1.85 26.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.00-1.85) 100.0 (26.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.85Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.196 , 0.267 0.193 , 0.195	Depositor DCC
R_{free} test set	3391 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7128	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: CL, 2PG, PEP, K, MG

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	0.42	0/3348	0.78	5/4530 (0.1%)
2	B	1.29	10/3314 (0.3%)	1.08	12/4480 (0.3%)
All	All	0.96	10/6662 (0.2%)	0.94	17/9010 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	163	ALA	N-CA	52.46	2.13	1.46
2	B	157	GLY	C-O	18.18	1.48	1.23
2	B	163	ALA	CA-CB	16.07	1.79	1.53
2	B	163	ALA	CA-C	-15.99	1.36	1.53
2	B	157	GLY	CA-C	14.69	1.72	1.51
2	B	157	GLY	N-CA	-14.00	1.25	1.45
2	B	156	GLY	C-N	-8.12	1.21	1.33
2	B	70	ASP	C-N	6.21	1.42	1.33
2	B	163	ALA	C-O	-5.48	1.17	1.23
2	B	272	TRP	NE1-CE2	-5.06	1.31	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	ALA	N-CA-C	-18.34	86.10	111.96
2	B	157	GLY	CA-C-O	-16.92	91.12	120.57
2	B	163	ALA	N-CA-CB	16.12	139.13	110.27
2	B	70	ASP	CA-C-N	-12.21	110.22	123.16
2	B	70	ASP	C-N-CA	-12.21	110.22	123.16
2	B	163	ALA	O-C-N	10.75	134.88	122.19
2	B	164	LEU	N-CA-C	-8.84	96.79	109.96
2	B	73	ALA	O-C-N	-7.88	112.25	121.32
2	B	13	SER	O-C-N	-7.74	112.14	122.43
1	A	383	ILE	O-C-N	-7.44	112.31	122.05
2	B	350	GLY	O-C-N	-6.92	115.08	122.56
1	A	244	GLY	O-C-N	-5.82	118.83	123.49
1	A	73	ALA	O-C-N	-5.79	114.66	121.32
2	B	208	VAL	N-CA-C	5.35	115.88	110.05
1	A	235	ALA	CA-C-N	5.18	131.63	121.06
1	A	235	ALA	C-N-CA	5.18	131.63	121.06
2	B	184	ARG	NE-CZ-NH2	5.14	123.82	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	LYS	Mainchain
2	B	396	LYS	Mainchain

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	3288	0	3292	58	0
2	B	3257	0	3265	99	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	10	0	2	0	0
4	B	10	0	2	0	0
5	A	11	0	4	0	0
5	B	11	0	4	3	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	274	0	0	1	0
8	B	261	0	0	4	0
All	All	7128	0	6569	151	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 11.

All (151) 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)
2:B:163:ALA:CA	2:B:163:ALA:CB	1.79	1.59
2:B:157:GLY:C	2:B:263:LYS:HE2	1.68	1.17
2:B:157:GLY:C	2:B:263:LYS:CE	2.22	1.13
2:B:163:ALA:CA	2:B:163:ALA:N	2.13	1.10
2:B:163:ALA:CA	2:B:263:LYS:HE3	1.86	1.04
2:B:157:GLY:C	2:B:263:LYS:NZ	2.24	0.95
2:B:163:ALA:HA	2:B:263:LYS:HE3	1.48	0.94
2:B:157:GLY:C	2:B:163:ALA:N	2.27	0.92
2:B:168:GLU:HB2	2:B:246:ASP:HB3	1.50	0.91
2:B:163:ALA:CB	2:B:163:ALA:HA	2.03	0.88
2:B:163:ALA:CA	2:B:263:LYS:CE	2.54	0.85
2:B:163:ALA:N	2:B:164:LEU:O	2.10	0.84
2:B:163:ALA:CB	2:B:163:ALA:C	2.50	0.83
2:B:140:LYS:HE2	2:B:391:ARG:NH2	2.01	0.76
2:B:163:ALA:N	2:B:163:ALA:C	2.45	0.74
2:B:233:LYS:O	2:B:233:LYS:HE3	1.87	0.73
2:B:196:LEU:HD23	2:B:199:LYS:HE2	1.70	0.73
2:B:163:ALA:CA	2:B:263:LYS:NZ	2.55	0.69
2:B:345:LYS:NZ	5:B:441[B]:2PG:H2	2.08	0.68
2:B:73:ALA:O	2:B:77:VAL:HG22	1.93	0.68
1:A:403:SER:HB2	2:B:404:GLU:HB3	1.74	0.67
1:A:140:LYS:HE3	1:A:391:ARG:NH2	2.09	0.67
2:B:259:ASP:OD2	2:B:262:PHE:HA	1.94	0.67
1:A:161:GLY:H	2:B:207:ASN:HD21	1.41	0.67
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.77	0.66
2:B:196:LEU:HA	2:B:199:LYS:HE2	1.78	0.66
2:B:249:SER:HA	2:B:252:PHE:CE2	2.32	0.65
2:B:274:THR:OG1	2:B:277:GLN:HG3	1.97	0.65
1:A:204:SER:HB2	8:A:1456:HOH:O	1.97	0.63
2:B:152:ASN:O	2:B:399:ALA:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:O	2:B:70:ASP:HB2	1.99	0.62
2:B:345:LYS:HZ3	5:B:441[B]:2PG:H2	1.64	0.61
1:A:273:LEU:HD22	1:A:277:GLN:HB3	1.82	0.61
1:A:404:GLU:HB3	2:B:403:SER:HB2	1.84	0.60
2:B:163:ALA:N	2:B:164:LEU:N	2.49	0.60
1:A:264:ASN:HD22	1:A:265:PRO:HD2	1.67	0.59
2:B:175:GLY:C	2:B:240:LYS:HD3	2.29	0.58
2:B:14:ARG:HH12	2:B:375:SER:HB2	1.69	0.56
1:A:252:PHE:HB3	1:A:262:PHE:CD2	2.40	0.56
2:B:260:LEU:HD11	2:B:281:LEU:HD22	1.88	0.56
1:A:326:ASN:OD1	1:A:328:LYS:HB2	2.05	0.55
1:A:7:ALA:HB2	1:A:68:VAL:HG11	1.87	0.55
1:A:278:LEU:HD12	1:A:281:LEU:HD23	1.88	0.55
2:B:17:PRO:HG2	2:B:59:LYS:O	2.08	0.54
1:A:154:LEU:HB3	1:A:169:PHE:HB2	1.89	0.54
2:B:313:ALA:CB	2:B:317:ILE:HD11	2.38	0.54
1:A:73:ALA:O	1:A:77:VAL:HG23	2.08	0.53
1:A:264:ASN:HD22	1:A:265:PRO:CD	2.21	0.53
2:B:362:SER:O	2:B:367:TRP:HB2	2.07	0.53
1:A:249:SER:HA	1:A:252:PHE:CE2	2.44	0.53
2:B:252:PHE:HB3	2:B:262:PHE:CD2	2.43	0.53
2:B:294:ILE:HD11	2:B:297:PRO:HB3	1.89	0.53
2:B:411:GLN:O	2:B:415:ILE:HG13	2.08	0.53
2:B:74:PRO:O	2:B:77:VAL:HG23	2.09	0.52
2:B:164:LEU:HD11	2:B:166:LEU:HB2	1.92	0.52
2:B:294:ILE:CD1	2:B:297:PRO:HB3	2.40	0.52
1:A:222:GLU:HG2	1:A:288:ARG:NH2	2.25	0.52
2:B:313:ALA:HB3	2:B:317:ILE:HD11	1.91	0.52
2:B:140:LYS:NZ	2:B:391:ARG:NH1	2.58	0.51
1:A:252:PHE:HB3	1:A:262:PHE:CG	2.46	0.51
2:B:163:ALA:HA	2:B:263:LYS:CE	2.30	0.50
2:B:14:ARG:HD3	2:B:210:ASP:OD2	2.11	0.50
1:A:37:GLY:HA3	1:A:374:ARG:NH2	2.27	0.49
1:A:374:ARG:O	1:A:377:GLU:HG2	2.13	0.49
2:B:46:LEU:HD23	2:B:103:SER:HA	1.92	0.49
2:B:41:GLY:O	2:B:44:GLU:HG3	2.12	0.49
2:B:196:LEU:HD23	2:B:199:LYS:CE	2.41	0.49
2:B:308:HIS:HA	2:B:311:LYS:HE3	1.94	0.49
1:A:343:LEU:HD11	1:A:396:LYS:HD3	1.95	0.48
2:B:175:GLY:O	2:B:240:LYS:HD3	2.13	0.48
1:A:294:ILE:HG13	1:A:315:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLY:HA3	1:A:405:ARG:HD2	1.94	0.48
2:B:403:SER:HA	2:B:406:LEU:HB2	1.96	0.48
1:A:44:GLU:CD	1:A:348:GLN:HG2	2.39	0.48
1:A:140:LYS:HG3	1:A:142:SER:H	1.78	0.48
2:B:296:ASP:HA	2:B:306:TRP:CH2	2.48	0.48
2:B:297:PRO:HD2	2:B:306:TRP:CH2	2.48	0.47
1:A:88:ALA:HA	1:A:91:ASP:HB2	1.96	0.47
1:A:281:LEU:HD11	1:A:285:LEU:HD11	1.96	0.47
2:B:33:ILE:CG2	2:B:378:THR:HG21	2.45	0.47
2:B:345:LYS:O	2:B:348:GLN:HB2	2.15	0.47
1:A:140:LYS:HE3	1:A:391:ARG:CZ	2.44	0.47
1:A:410:ASN:O	1:A:413:LEU:HB2	2.14	0.47
1:A:373:HIS:CG	1:A:397:THR:HA	2.50	0.46
2:B:101:ASN:ND2	8:B:1270:HOH:O	2.47	0.46
2:B:141:THR:HB	2:B:144:TYR:CE2	2.51	0.46
1:A:130:TYR:CE1	1:A:419:LEU:HD21	2.51	0.46
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.51	0.46
1:A:401:ALA:O	1:A:402:ARG:HB2	2.16	0.46
2:B:267:SER:OG	2:B:272:TRP:NE1	2.47	0.46
1:A:404:GLU:HB3	2:B:403:SER:CB	2.46	0.46
1:A:434:ASP:OD1	1:A:435:LYS:HD3	2.15	0.46
2:B:325:THR:HG22	2:B:325:THR:O	2.16	0.46
2:B:42:VAL:HG12	2:B:300:GLU:CD	2.41	0.46
2:B:269:LYS:HA	2:B:272:TRP:CE2	2.51	0.45
2:B:303:TRP:CZ3	2:B:322:LEU:HD11	2.51	0.45
2:B:345:LYS:NZ	8:B:1419:HOH:O	2.50	0.45
1:A:141:THR:HG22	1:A:144:TYR:CE1	2.51	0.45
1:A:296:ASP:OD2	1:A:320:ASP:HB3	2.16	0.45
1:A:15:GLY:O	2:B:191:HIS:HE1	1.99	0.45
2:B:296:ASP:OD2	2:B:320:ASP:HB3	2.16	0.45
1:A:34:VAL:HG13	1:A:111:LEU:HD23	1.98	0.45
2:B:398:GLY:HA3	2:B:405:ARG:HD2	1.99	0.45
2:B:7:ALA:HB2	2:B:68:VAL:HG11	1.98	0.45
1:A:185:ILE:HG23	1:A:237:HIS:CD2	2.52	0.45
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.99	0.45
1:A:152:ASN:O	1:A:399:ALA:HB2	2.17	0.44
2:B:27:LYS:HE2	2:B:27:LYS:HB3	1.81	0.44
1:A:221:ALA:O	1:A:224:ALA:N	2.50	0.44
2:B:127:VAL:CG1	2:B:131:LYS:HE3	2.47	0.44
1:A:306:TRP:HB3	1:A:338:ALA:HB1	1.98	0.44
1:A:226:ASP:HA	1:A:229:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:NZ	8:B:1298:HOH:O	2.44	0.43
2:B:218:ILE:HG23	2:B:223:GLU:OE1	2.18	0.43
2:B:277:GLN:O	2:B:280:ASP:HB2	2.18	0.43
1:A:403:SER:CB	2:B:404:GLU:HB3	2.46	0.43
1:A:20:GLU:OE1	1:A:31:ARG:HD3	2.17	0.43
1:A:195:SER:O	1:A:199:LYS:HG3	2.18	0.43
2:B:260:LEU:CD1	2:B:281:LEU:HD22	2.49	0.43
1:A:325:THR:HG22	1:A:325:THR:O	2.19	0.43
1:A:151:LEU:O	1:A:170:MET:HA	2.19	0.43
2:B:140:LYS:HZ3	2:B:391:ARG:NH1	2.17	0.43
2:B:275:GLY:N	2:B:276:PRO:HD2	2.34	0.42
2:B:406:LEU:HD13	2:B:406:LEU:HA	1.85	0.42
1:A:349:ILE:HG12	1:A:354:GLU:HB3	2.01	0.42
2:B:247:CYS:HB2	2:B:296:ASP:O	2.19	0.42
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.54	0.42
2:B:273:LEU:HA	2:B:277:GLN:OE1	2.19	0.42
2:B:384:ALA:O	2:B:387:VAL:HG12	2.18	0.42
1:A:249:SER:HA	1:A:252:PHE:CZ	2.55	0.42
1:A:125:LYS:O	1:A:126:ASN:HB2	2.19	0.42
2:B:142:SER:HA	2:B:143:PRO:HA	1.80	0.42
2:B:347:ASN:OD1	2:B:374:ARG:HD3	2.20	0.42
2:B:164:LEU:O	2:B:164:LEU:HG	2.20	0.41
1:A:252:PHE:HB2	1:A:259:ASP:O	2.21	0.41
2:B:147:PRO:HA	2:B:393:GLY:C	2.45	0.41
1:A:264:ASN:ND2	1:A:266:ASN:H	2.18	0.41
1:A:295:GLU:OE2	1:A:343:LEU:HD22	2.19	0.41
2:B:345:LYS:CE	5:B:441[B]:2PG:H2	2.50	0.41
1:A:142:SER:HA	1:A:143:PRO:HA	1.82	0.41
2:B:199:LYS:HG3	8:B:1497:HOH:O	2.19	0.41
1:A:286:MET:HE3	1:A:315:ILE:HG12	2.02	0.41
2:B:73:ALA:HB3	2:B:74:PRO:CD	2.51	0.41
2:B:252:PHE:HB3	2:B:262:PHE:CG	2.56	0.41
2:B:298:PHE:HB2	2:B:306:TRP:CD1	2.56	0.41
2:B:324:VAL:HG23	2:B:324:VAL:O	2.21	0.41
2:B:151:LEU:O	2:B:170:MET:HA	2.21	0.40
2:B:344:LEU:HD21	2:B:355:SER:HB3	2.02	0.40
2:B:373:HIS:ND1	2:B:405:ARG:NH1	2.70	0.40
2:B:72:ILE:HA	2:B:96:LEU:HD21	2.04	0.40
2:B:198:LYS:HB2	2:B:198:LYS:HE2	1.86	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	434/436 (100%)	423 (98%)	10 (2%)	1 (0%)	43	31
2	B	424/436 (97%)	410 (97%)	12 (3%)	2 (0%)	24	13
All	All	858/872 (98%)	833 (97%)	22 (3%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
2	B	268	ASP
2	B	402	ARG

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	343/343 (100%)	331 (96%)	12 (4%)	32	16
2	B	341/344 (99%)	321 (94%)	20 (6%)	18	5
All	All	684/687 (100%)	652 (95%)	32 (5%)	23	9

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

Mol	Chain	Res	Type
1	A	27	LYS
1	A	33	ILE
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	177	LYS
1	A	223	GLU
1	A	270	SER
1	A	281	LEU
1	A	311	LYS
1	A	312	THR
1	A	347	ASN
1	A	392	THR
1	A	406	LEU
2	B	53	LYS
2	B	77	VAL
2	B	140	LYS
2	B	155	ASN
2	B	164	LEU
2	B	194	LYS
2	B	198	LYS
2	B	222	GLU
2	B	233	LYS
2	B	238	ASP
2	B	240	LYS
2	B	267	SER
2	B	269	LYS
2	B	271	LYS
2	B	284	SER
2	B	337	LYS
2	B	347	ASN
2	B	392	THR
2	B	406	LEU
2	B	436	LEU

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	152	ASN
1	A	167	GLN
1	A	264	ASN
1	A	266	ASN
1	A	422	ASN
2	B	101	ASN
2	B	152	ASN
2	B	207	ASN

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Mol	Chain	Res	Type
2	B	308	HIS
2	B	422	ASN

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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$
5	2PG	B	441[B]	3	9,10,10	1.16	1 (11%)	12,14,14	1.28	2 (16%)
5	2PG	A	441[B]	3	9,10,10	1.16	1 (11%)	12,14,14	1.29	2 (16%)
4	PEP	B	440[A]	3	9,9,9	2.15	2 (22%)	11,13,13	1.47	3 (27%)
4	PEP	A	440[A]	3	9,9,9	2.13	2 (22%)	11,13,13	1.42	3 (27%)

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
5	2PG	B	441[B]	3	-	0/11/11/11	-
5	2PG	A	441[B]	3	-	1/11/11/11	-
4	PEP	B	440[A]	3	-	0/9/9/9	-
4	PEP	A	440[A]	3	-	0/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	440[A]	PEP	C2-C1	4.70	1.54	1.49
4	A	440[A]	PEP	C2-C1	4.66	1.53	1.49
4	B	440[A]	PEP	C3-C2	2.88	1.39	1.31
4	A	440[A]	PEP	C3-C2	2.85	1.39	1.31
5	A	441[B]	2PG	O2-C1	-2.18	1.23	1.30
5	B	441[B]	2PG	O2-C1	-2.16	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	441[B]	2PG	O2-C1-C2	3.00	120.51	112.71
5	A	441[B]	2PG	O2-C1-C2	2.93	120.32	112.71
4	B	440[A]	PEP	O2'-C1-C2	2.62	118.38	113.91
4	A	440[A]	PEP	O2'-C1-C2	2.53	118.22	113.91
4	B	440[A]	PEP	O2-C2-C3	-2.46	120.14	124.85
4	B	440[A]	PEP	O1-C1-C2	-2.38	118.20	121.79
4	A	440[A]	PEP	O2-C2-C3	-2.38	120.30	124.85
4	A	440[A]	PEP	O1-C1-C2	-2.31	118.30	121.79
5	A	441[B]	2PG	O2-C1-O1	-2.25	118.96	124.08
5	B	441[B]	2PG	O2-C1-O1	-2.20	119.09	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	441[B]	2PG	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	441[B]	2PG	3	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	436/436 (100%)	-0.11	8 (1%) 67 71	7, 15, 33, 48	0
2	B	430/436 (98%)	0.09	18 (4%) 40 44	8, 17, 40, 67	0
All	All	866/872 (99%)	-0.01	26 (3%) 52 56	7, 16, 37, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	GLY	8.6
1	A	268	ASP	8.1
2	B	163	ALA	7.8
2	B	271	LYS	6.6
2	B	269	LYS	4.3
1	A	222	GLU	4.0
2	B	260	LEU	3.7
2	B	335	GLU	3.7
2	B	140	LYS	3.6
1	A	281	LEU	3.1
1	A	276	PRO	3.0
1	A	271	LYS	3.0
2	B	274	THR	2.9
2	B	428	GLU	2.9
2	B	164	LEU	2.9
2	B	281	LEU	2.6
2	B	255	ASP	2.6
2	B	272	TRP	2.6
2	B	422	ASN	2.5
2	B	270	SER	2.4
2	B	284	SER	2.4
1	A	92	PHE	2.2
1	A	270	SER	2.2
2	B	436	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	311	LYS	2.2
1	A	304	GLU	2.1

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 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(Å ²)	Q<0.9
3	MG	B	439	1/1	0.83	0.23	39,39,39,39	0
7	K	B	960	1/1	0.87	0.18	48,48,48,48	0
3	MG	A	439	1/1	0.96	0.03	15,15,15,15	0
5	2PG	B	441[B]	11/11	0.96	0.06	10,14,18,23	11
3	MG	B	438	1/1	0.96	0.06	12,12,12,12	0
6	CL	B	950	1/1	0.97	0.05	18,18,18,18	0
3	MG	A	438	1/1	0.97	0.03	10,10,10,10	0
4	PEP	A	440[A]	10/10	0.98	0.05	4,10,12,12	10
4	PEP	B	440[A]	10/10	0.98	0.05	10,15,16,20	10
5	2PG	A	441[B]	11/11	0.98	0.05	2,8,12,13	11

6.5 Other polymers [i](#)

There are no such residues in this entry.