



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:37 PM UTC

PDB ID : 2ZYR / pdb_00002zyr
Title : A. Fulgidus lipase with fatty acid fragment and magnesium
Authors : Chen, C.K.; Ko, T.P.; Guo, R.T.; Wang, A.H.
Deposited on : 2009-01-28
Resolution : 1.77 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

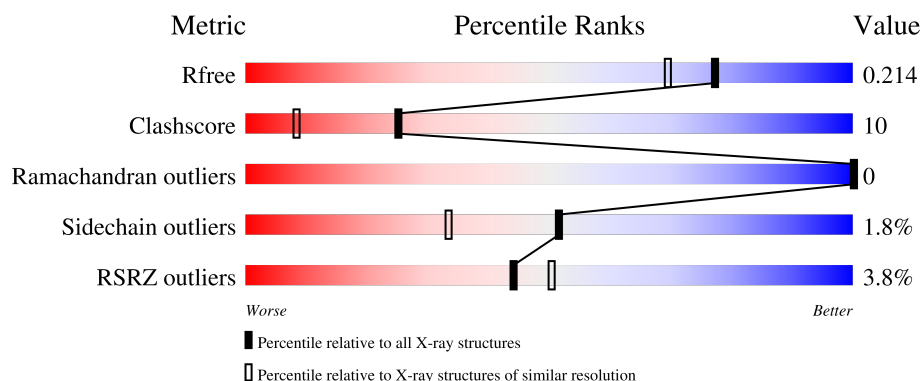
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	484	2% 77% 18% • •
1	B	484	5% 73% 19% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8535 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.

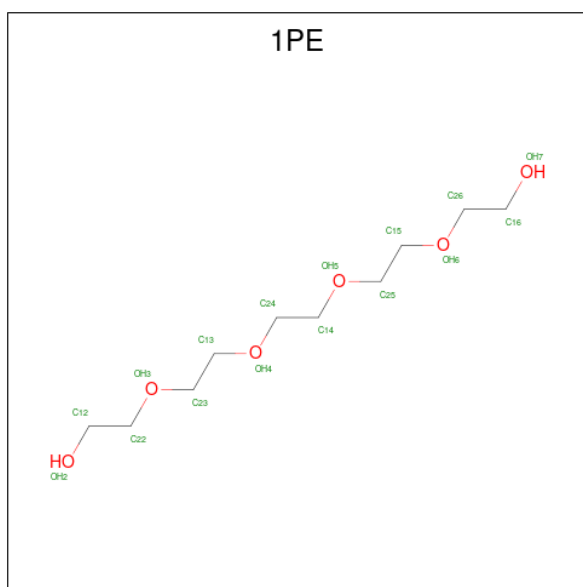
- Molecule 1 is a protein called Lipase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3660	2357	606	685	12			
1	B	454	Total	C	N	O	S	0	0	0
			3586	2310	593	671	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	VAL	-	expression tag	UNP O28511
A	476	ASP	-	expression tag	UNP O28511
A	477	LYS	-	expression tag	UNP O28511
A	478	LEU	-	expression tag	UNP O28511
A	479	ALA	-	expression tag	UNP O28511
A	480	ALA	-	expression tag	UNP O28511
A	481	ALA	-	expression tag	UNP O28511
A	482	LEU	-	expression tag	UNP O28511
A	483	GLU	-	expression tag	UNP O28511
A	484	HIS	-	expression tag	UNP O28511
B	475	VAL	-	expression tag	UNP O28511
B	476	ASP	-	expression tag	UNP O28511
B	477	LYS	-	expression tag	UNP O28511
B	478	LEU	-	expression tag	UNP O28511
B	479	ALA	-	expression tag	UNP O28511
B	480	ALA	-	expression tag	UNP O28511
B	481	ALA	-	expression tag	UNP O28511
B	482	LEU	-	expression tag	UNP O28511
B	483	GLU	-	expression tag	UNP O28511
B	484	HIS	-	expression tag	UNP O28511

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			13	8	5		

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

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

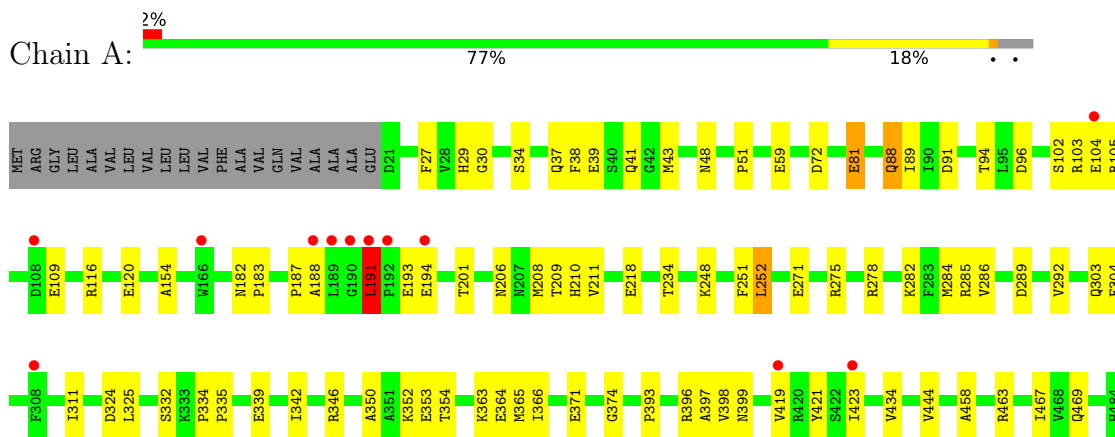
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	697	Total	O	0	0
			697	697		
4	B	558	Total	O	0	0
			558	558		

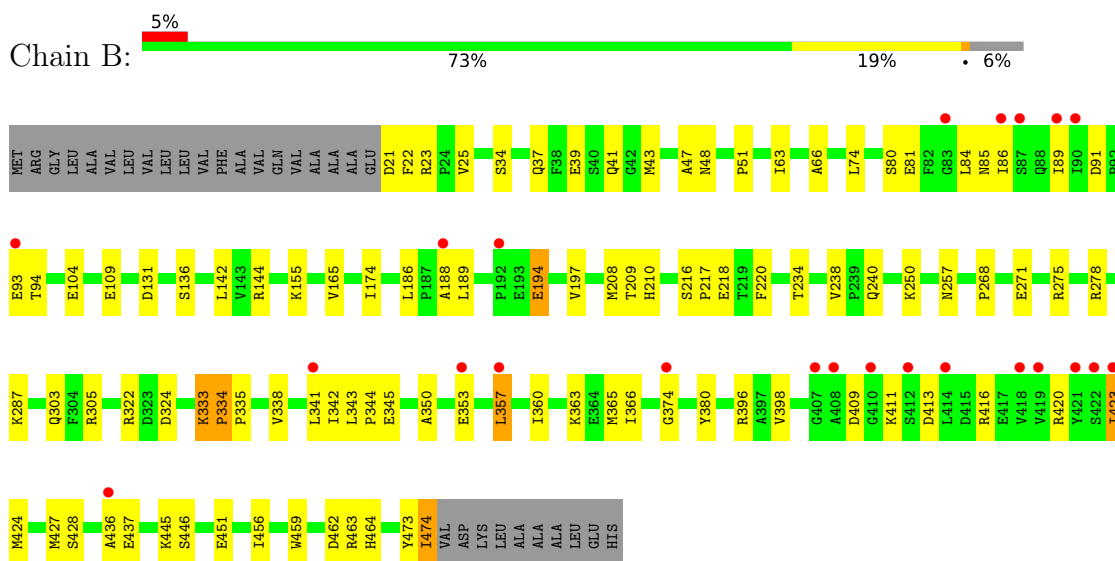
3 Residue-property plots [i](#)

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: Lipase, putative



- Molecule 1: Lipase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.29Å 106.67Å 175.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 30.00 – 1.77	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-1.77) 93.7 (30.00-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.214 0.178 , 0.214	Depositor DCC
R_{free} test set	4527 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8535	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1PE

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	1.09	8/3748 (0.2%)	1.18	15/5088 (0.3%)
1	B	0.99	6/3673 (0.2%)	1.19	19/4986 (0.4%)
All	All	1.04	14/7421 (0.2%)	1.18	34/10074 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	VAL	CA-CB	7.84	1.61	1.54
1	B	165	VAL	CA-CB	6.94	1.61	1.54
1	B	360	ILE	CA-CB	6.64	1.62	1.54
1	A	154	ALA	CA-CB	6.59	1.64	1.53
1	A	365	MET	SD-CE	6.09	1.94	1.79
1	A	51	PRO	CA-C	5.56	1.59	1.52
1	A	43	MET	SD-CE	-5.37	1.66	1.79
1	A	458	ALA	CA-CB	5.35	1.59	1.52
1	A	284	MET	SD-CE	-5.26	1.66	1.79
1	A	444	VAL	CA-CB	5.15	1.60	1.54
1	B	66	ALA	CA-CB	5.13	1.61	1.53
1	B	25	VAL	CA-CB	5.12	1.60	1.54
1	B	334	PRO	CA-C	5.07	1.56	1.52
1	B	365	MET	SD-CE	5.04	1.92	1.79

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	VAL	N-CA-C	10.45	118.32	107.76
1	A	334	PRO	N-CA-C	-9.70	98.87	110.70
1	A	210	HIS	N-CA-C	8.78	121.73	111.02
1	B	374	GLY	N-CA-C	8.49	127.04	115.32
1	B	210	HIS	N-CA-C	7.31	119.94	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	PRO	N-CA-C	-7.26	99.82	111.14
1	B	51	PRO	N-CA-C	-7.19	99.93	111.14
1	B	398	VAL	N-CA-C	7.13	117.67	108.12
1	B	363	LYS	N-CA-C	-6.63	96.67	110.80
1	B	268	PRO	N-CA-C	-6.58	100.85	111.19
1	A	398	VAL	N-CA-C	6.47	116.80	108.12
1	B	436	ALA	N-CA-C	6.32	120.48	113.21
1	A	363	LYS	N-CA-C	-6.08	97.85	110.80
1	A	81	GLU	N-CA-C	6.06	118.38	111.11
1	A	201	THR	N-CA-C	-5.98	100.09	109.25
1	B	446	SER	N-CA-C	5.82	119.39	110.20
1	A	285	ARG	N-CA-C	-5.69	100.71	109.76
1	B	197	VAL	N-CA-C	-5.64	99.61	107.80
1	A	365	MET	N-CA-C	-5.46	100.28	108.96
1	A	419	VAL	N-CA-C	5.44	118.67	111.17
1	B	257	ASN	N-CA-C	5.42	119.47	112.86
1	A	251	PHE	N-CA-C	-5.37	99.98	108.73
1	B	436	ALA	CA-C-N	-5.37	114.25	122.62
1	B	436	ALA	C-N-CA	-5.37	114.25	122.62
1	A	188	ALA	N-CA-C	5.36	118.96	111.30
1	B	91	ASP	CA-C-N	5.32	125.39	119.32
1	B	91	ASP	C-N-CA	5.32	125.39	119.32
1	B	380	TYR	N-CA-C	5.31	117.89	109.24
1	B	456	ILE	N-CA-C	5.13	114.61	108.45
1	B	142	LEU	N-CA-C	5.12	116.94	111.36
1	A	289	ASP	N-CA-C	5.12	117.31	110.35
1	B	194	GLU	N-CA-C	5.12	116.72	108.32
1	A	191	LEU	N-CA-C	5.11	118.28	108.97
1	A	374	GLY	N-CA-C	5.07	122.31	115.32

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	3660	0	3615	67	0
1	B	3586	0	3539	76	0
2	A	16	0	22	0	0
2	B	13	0	17	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	697	0	0	17	0
4	B	558	0	0	24	0
All	All	8535	0	7193	141	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 10.

All (141) 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:287:LYS:HE2	4:B:1031:HOH:O	1.55	1.05
1:A:105:ARG:O	1:A:109:GLU:HG3	1.64	0.97
1:A:193:GLU:HG3	4:A:1087:HOH:O	1.77	0.85
1:B:423:ILE:HD11	4:B:1123:HOH:O	1.82	0.79
1:A:120:GLU:HG3	4:A:1054:HOH:O	1.84	0.77
1:B:85:ASN:HB2	4:B:1121:HOH:O	1.83	0.77
1:B:287:LYS:HD3	4:B:1027:HOH:O	1.84	0.77
1:B:85:ASN:HB3	4:B:499:HOH:O	1.84	0.77
1:B:420:ARG:HD3	4:B:672:HOH:O	1.84	0.77
1:B:445:LYS:HG2	1:B:451:GLU:HG2	1.67	0.76
1:A:194:GLU:HA	4:A:738:HOH:O	1.85	0.76
1:A:463:ARG:HD3	4:A:790:HOH:O	1.90	0.72
1:A:282:LYS:HG3	1:A:292:VAL:HG21	1.73	0.71
1:A:271:GLU:H	1:A:271:GLU:CD	1.96	0.71
1:B:338:VAL:HG12	1:B:424:MET:HE2	1.70	0.71
1:A:354:THR:HG21	4:A:811:HOH:O	1.91	0.70
1:A:423:ILE:HG23	4:A:1016:HOH:O	1.89	0.70
1:A:423:ILE:CG2	4:A:1016:HOH:O	2.40	0.69
1:A:103:ARG:HH11	1:A:103:ARG:HG2	1.56	0.69
1:B:39:GLU:OE2	4:B:513:HOH:O	2.10	0.69
1:B:271:GLU:HG2	4:B:641:HOH:O	1.92	0.69
1:A:72:ASP:OD2	1:A:103:ARG:NH2	2.26	0.68
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.08	0.68
1:B:462:ASP:OD2	1:B:463:ARG:HG3	1.95	0.67
1:A:34:SER:H	1:A:37:GLN:HE22	1.43	0.67
1:A:89:ILE:O	1:A:89:ILE:HG22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD21	1:B:189:LEU:HD12	1.75	0.66
1:B:437:GLU:O	4:B:947:HOH:O	2.14	0.66
1:A:88:GLN:HG2	1:A:89:ILE:HD13	1.78	0.65
1:A:120:GLU:CG	4:A:1054:HOH:O	2.43	0.65
1:A:102:SER:HB3	1:A:105:ARG:HB3	1.79	0.64
1:B:424:MET:HB3	1:B:427:MET:CE	2.27	0.64
1:B:240:GLN:HG2	1:B:322:ARG:HA	1.80	0.64
1:A:286:VAL:HG21	1:A:304:PHE:HE1	1.62	0.64
1:B:209:THR:HG21	1:B:366:ILE:HD11	1.80	0.64
1:B:34:SER:H	1:B:37:GLN:HE22	1.46	0.62
1:B:338:VAL:CG1	1:B:424:MET:HE2	2.29	0.62
1:B:48:ASN:HD21	1:B:234:THR:H	1.47	0.61
1:A:371:GLU:O	1:A:371:GLU:CD	2.44	0.61
1:B:21:ASP:CG	1:B:22:PHE:H	2.09	0.61
1:B:338:VAL:HG12	1:B:424:MET:CE	2.31	0.60
1:A:278:ARG:HD3	4:A:779:HOH:O	2.01	0.60
1:A:350:ALA:O	1:A:354:THR:HG23	2.02	0.59
1:A:282:LYS:HG3	1:A:292:VAL:CG2	2.32	0.58
1:B:21:ASP:N	4:B:705:HOH:O	2.36	0.58
1:B:424:MET:CE	1:B:427:MET:HE1	2.34	0.58
1:B:93:GLU:HG3	4:B:787:HOH:O	2.04	0.57
1:B:424:MET:HB3	1:B:427:MET:HE3	1.86	0.57
1:B:275:ARG:HH22	1:B:303:GLN:NE2	2.03	0.56
1:A:423:ILE:O	1:A:423:ILE:HG12	2.06	0.56
1:B:81:GLU:HG2	1:B:188:ALA:HB1	1.88	0.56
1:B:462:ASP:CG	1:B:463:ARG:HG3	2.31	0.55
1:A:208:MET:HE1	1:A:218:GLU:HB2	1.87	0.55
1:B:74:LEU:HD23	1:B:144:ARG:HG2	1.89	0.55
1:B:473:TYR:OH	4:B:1202:HOH:O	2.18	0.54
1:A:206:ASN:ND2	4:A:733:HOH:O	2.40	0.53
1:B:80:SER:O	1:B:84:LEU:HG	2.07	0.53
1:A:286:VAL:CG2	1:A:304:PHE:HE1	2.21	0.53
1:B:357:LEU:N	1:B:357:LEU:HD23	2.23	0.53
1:A:396:ARG:NH2	4:A:1152:HOH:O	2.41	0.53
1:B:424:MET:HE3	1:B:427:MET:HE1	1.90	0.53
1:A:467:ILE:HD12	1:A:467:ILE:N	2.25	0.52
1:A:81:GLU:HB3	4:A:979:HOH:O	2.09	0.52
1:B:186:LEU:CD2	1:B:189:LEU:HD12	2.40	0.51
1:A:29:HIS:HD2	1:A:30:GLY:O	1.94	0.51
1:B:208:MET:HE1	1:B:216:SER:OG	2.11	0.51
1:B:333:LYS:HG3	1:B:334:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:HD21	1:A:234:THR:H	1.58	0.50
1:B:341:LEU:HD13	1:B:420:ARG:HB3	1.93	0.50
1:A:34:SER:H	1:A:37:GLN:NE2	2.09	0.50
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.73	0.50
1:B:474:ILE:HG22	4:B:677:HOH:O	2.12	0.50
1:A:248:LYS:HB2	1:A:325:LEU:HA	1.95	0.49
1:B:343:LEU:N	1:B:344:PRO:CD	2.75	0.49
1:A:275:ARG:HH22	1:A:303:GLN:NE2	2.10	0.49
1:B:423:ILE:HD12	1:B:423:ILE:H	1.77	0.49
1:B:396:ARG:NH1	1:B:428:SER:OG	2.46	0.49
1:A:88:GLN:O	1:A:88:GLN:HG3	2.13	0.48
1:A:346:ARG:NH2	4:A:794:HOH:O	2.43	0.48
1:A:29:HIS:CE1	1:A:59:GLU:HA	2.49	0.48
1:B:89:ILE:CG2	1:B:423:ILE:HD13	2.44	0.48
1:B:39:GLU:OE1	1:B:324:ASP:OD2	2.33	0.47
1:B:342:ILE:HA	1:B:420:ARG:HH21	1.79	0.47
1:B:218:GLU:OE2	1:B:218:GLU:N	2.47	0.47
1:B:217:PRO:HG2	1:B:218:GLU:OE2	2.15	0.47
1:A:103:ARG:CD	4:A:1003:HOH:O	2.63	0.46
1:A:311:ILE:HG13	1:A:346:ARG:NH1	2.30	0.46
1:B:94:THR:HG21	1:B:335:PRO:HB3	1.96	0.46
1:A:209:THR:HG21	1:A:366:ILE:HD11	1.98	0.46
1:B:23:ARG:HD2	1:B:131:ASP:CG	2.41	0.46
1:B:34:SER:H	1:B:37:GLN:NE2	2.12	0.46
1:B:413:ASP:OD1	1:B:416:ARG:HB3	2.17	0.45
1:B:459:TRP:HB3	1:B:464:HIS:CG	2.51	0.45
1:B:463:ARG:NH1	4:B:1192:HOH:O	2.49	0.45
1:A:191:LEU:HD12	4:A:1087:HOH:O	2.16	0.45
1:A:94:THR:HG21	1:A:335:PRO:HB3	1.98	0.45
1:B:109:GLU:CD	4:B:817:HOH:O	2.59	0.45
1:A:39:GLU:OE1	1:A:324:ASP:OD2	2.35	0.45
1:A:89:ILE:O	1:A:89:ILE:CG2	2.64	0.44
1:A:252:LEU:H	1:A:252:LEU:HD23	1.82	0.44
1:B:155:LYS:NZ	4:B:751:HOH:O	2.50	0.44
1:B:250:LYS:HE3	4:B:877:HOH:O	2.16	0.44
1:B:305:ARG:NH2	4:B:1015:HOH:O	2.50	0.44
1:A:342:ILE:HG23	1:A:421:TYR:OH	2.18	0.44
1:B:81:GLU:HG2	1:B:188:ALA:CB	2.48	0.44
1:B:41:GLN:HA	1:B:41:GLN:OE1	2.18	0.44
1:B:345:GLU:CD	1:B:420:ARG:HH22	2.26	0.44
1:A:286:VAL:HG21	1:A:304:PHE:CE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE2	4:B:817:HOH:O	2.21	0.43
1:A:88:GLN:HE21	1:A:88:GLN:HB2	1.62	0.43
1:A:116:ARG:O	1:A:120:GLU:HG3	2.18	0.43
1:A:27:PHE:CD2	1:A:38:PHE:HB2	2.54	0.43
1:A:364:GLU:HG2	1:A:397:ALA:HA	2.01	0.43
1:B:136:SER:OG	4:B:870:HOH:O	2.04	0.43
1:B:305:ARG:HD3	4:B:720:HOH:O	2.18	0.43
1:B:474:ILE:H	1:B:474:ILE:HG12	1.58	0.42
1:A:393:PRO:HG2	1:A:396:ARG:CG	2.50	0.42
1:B:63:ILE:HG23	1:B:86:ILE:HG21	2.01	0.42
1:B:43:MET:HE1	4:B:1202:HOH:O	2.19	0.42
1:B:47:ALA:HB2	4:B:853:HOH:O	2.20	0.42
1:A:191:LEU:C	1:B:278:ARG:HD3	2.45	0.41
1:A:393:PRO:HG2	1:A:396:ARG:HG3	2.02	0.41
1:A:29:HIS:HE1	1:A:59:GLU:HA	1.84	0.41
1:A:211:VAL:HB	1:A:399:ASN:HD21	1.85	0.41
1:A:463:ARG:CD	4:A:790:HOH:O	2.60	0.41
1:A:352:LYS:NZ	1:A:353:GLU:OE2	2.45	0.41
1:B:41:GLN:OE1	1:B:220:PHE:HB2	2.21	0.41
1:A:332:SER:CB	1:A:339:GLU:HB2	2.51	0.41
1:A:211:VAL:CB	1:A:399:ASN:HD21	2.33	0.41
1:B:345:GLU:OE1	1:B:420:ARG:NH2	2.54	0.41
1:B:424:MET:HE2	1:B:427:MET:HE1	2.02	0.41
1:A:34:SER:N	1:A:37:GLN:HE22	2.12	0.41
1:A:182:ASN:HA	1:A:183:PRO:HD2	1.95	0.41
1:A:194:GLU:CA	4:A:738:HOH:O	2.56	0.41
1:B:21:ASP:CG	1:B:22:PHE:N	2.77	0.41
1:A:41:GLN:HA	1:A:41:GLN:OE1	2.21	0.41
1:B:104:GLU:HG2	4:B:883:HOH:O	2.20	0.41
1:B:409:ASP:OD2	1:B:411:LYS:HB2	2.21	0.40
1:A:191:LEU:O	1:B:278:ARG:HD3	2.20	0.40
1:B:86:ILE:O	1:B:89:ILE:HG12	2.21	0.40
1:B:350:ALA:O	1:B:353:GLU:N	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/484 (96%)	453 (98%)	9 (2%)	0	100	100
1	B	452/484 (93%)	444 (98%)	8 (2%)	0	100	100
All	All	914/968 (94%)	897 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	393/407 (97%)	385 (98%)	8 (2%)	48	29
1	B	386/407 (95%)	380 (98%)	6 (2%)	55	38
All	All	779/814 (96%)	765 (98%)	14 (2%)	51	33

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	91	ASP
1	A	96	ASP
1	A	104	GLU
1	A	187	PRO
1	A	191	LEU
1	A	252	LEU
1	A	469	GLN

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Mol	Chain	Res	Type
1	B	174	ILE
1	B	194	GLU
1	B	333	LYS
1	B	357	LEU
1	B	423	ILE
1	B	474	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	37	GLN
1	A	48	ASN
1	A	88	GLN
1	A	240	GLN
1	A	303	GLN
1	A	399	ASN
1	A	469	GLN
1	A	484	HIS
1	B	37	GLN
1	B	48	ASN
1	B	88	GLN
1	B	206	ASN
1	B	303	GLN
1	B	399	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 7 ligands modelled in this entry, 5 are 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
2	1PE	A	500	-	15,15,15	1.05	1 (6%)	14,14,14	0.40	0
2	1PE	B	500	-	12,12,15	0.94	0	11,11,14	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
2	1PE	A	500	-	-	6/13/13/13	-
2	1PE	B	500	-	-	5/10/10/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	1PE	C24-C14	2.16	1.59	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	1PE	OH5-C14-C24-OH4
2	A	500	1PE	OH7-C16-C26-OH6
2	B	500	1PE	OH4-C13-C23-OH3
2	B	500	1PE	OH2-C12-C22-OH3
2	A	500	1PE	OH6-C15-C25-OH5
2	A	500	1PE	C24-C14-OH5-C25
2	A	500	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
2	B	500	1PE	C23-C13-OH4-C24
2	B	500	1PE	OH5-C14-C24-OH4
2	A	500	1PE	C16-C26-OH6-C15
2	B	500	1PE	C14-C24-OH4-C13

There are no ring outliers.

No monomer is involved in short contacts.

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	464/484 (95%)	-0.02	12 (2%) 57 65	14, 23, 38, 73	0
1	B	454/484 (93%)	0.28	23 (5%) 33 39	15, 28, 51, 66	0
All	All	918/968 (94%)	0.13	35 (3%) 44 50	14, 25, 47, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	LEU	7.2
1	A	191	LEU	5.3
1	A	188	ALA	4.6
1	B	407	GLY	4.4
1	A	192	PRO	4.3
1	B	83	GLY	4.0
1	A	190	GLY	3.9
1	B	408	ALA	3.7
1	B	374	GLY	3.3
1	B	422	SER	3.1
1	B	86	ILE	3.0
1	A	423	ILE	3.0
1	B	188	ALA	3.0
1	B	436	ALA	2.9
1	A	104	GLU	2.9
1	B	341	LEU	2.8
1	B	89	ILE	2.8
1	B	410	GLY	2.6
1	A	108	ASP	2.6
1	B	412	SER	2.6
1	A	419	VAL	2.5
1	B	90	ILE	2.5
1	B	414	LEU	2.5
1	B	423	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	PRO	2.4
1	A	166	TRP	2.4
1	B	421	TYR	2.3
1	B	93	GLU	2.2
1	B	419	VAL	2.1
1	B	357	LEU	2.1
1	A	194	GLU	2.1
1	A	308	PHE	2.1
1	B	418	VAL	2.0
1	B	353	GLU	2.0
1	B	87	SER	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 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
2	1PE	A	500	16/16	0.90	0.09	29,36,43,43	0
2	1PE	B	500	13/16	0.90	0.11	31,39,48,51	0
3	MG	B	2004	1/1	0.94	0.08	36,36,36,36	0
3	MG	A	2003	1/1	0.95	0.07	22,22,22,22	0
3	MG	A	2001	1/1	0.96	0.06	31,31,31,31	0
3	MG	B	2005	1/1	0.96	0.08	38,38,38,38	0
3	MG	A	2002	1/1	0.97	0.05	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.