



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:27 PM UTC

PDB ID : 5EY5 / pdb_00005ey5
Title : LBCATS
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Deposited on : 2015-11-24
Resolution : 1.97 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

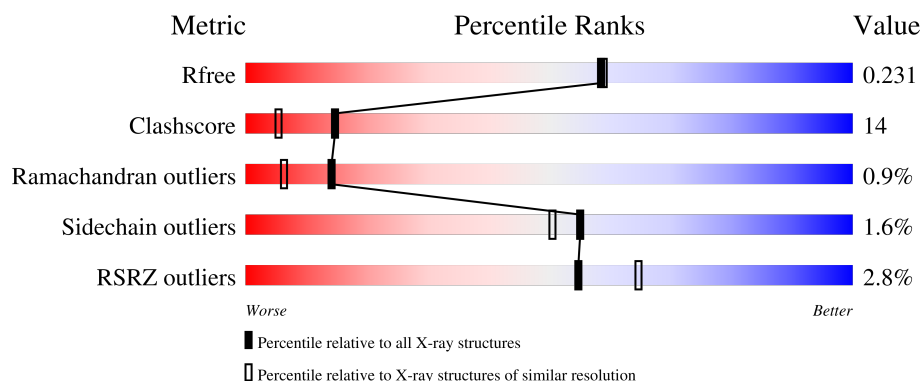
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	273	4% 68% 24% ...
1	C	273	7% 59% 28% 10%
2	B	399	79% 17% .
2	D	399	2% 72% 24% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9975 atoms, of which 8 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.

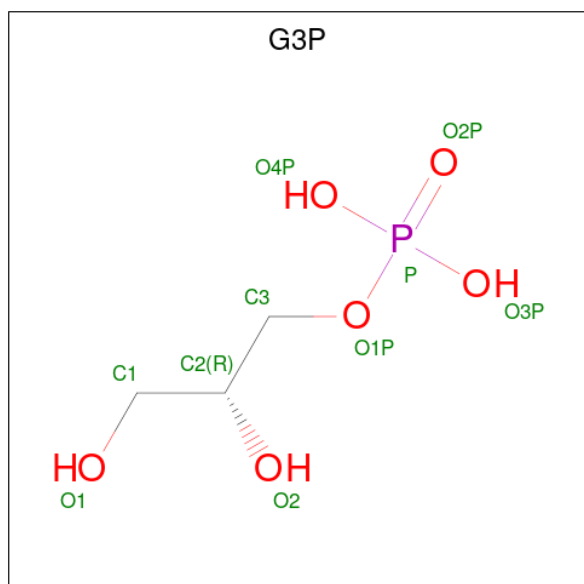
- Molecule 1 is a protein called LBCATS-a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1920	1227	324	364	5			
1	C	245	Total	C	N	O	S	0	0	0
			1765	1132	290	339	4			

- Molecule 2 is a protein called LBCA-b.

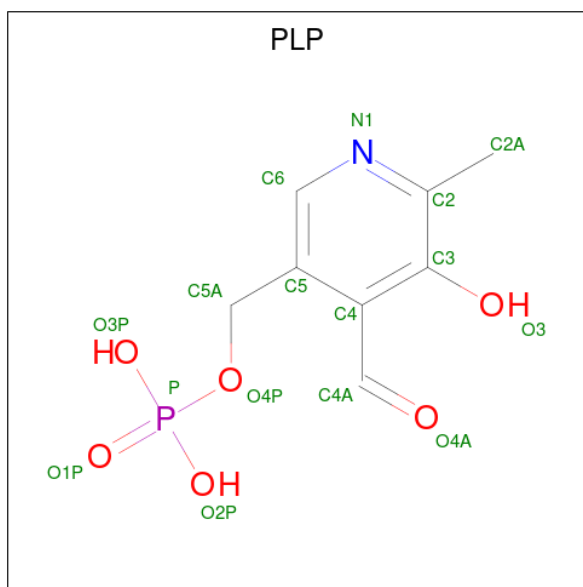
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	383	Total	C	N	O	S	0	0	0
			2916	1836	506	561	13			
2	D	383	Total	C	N	O	S	0	0	0
			2915	1834	505	563	13			

- Molecule 3 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		
4	D	1	Total	C	N	O	P		0	0
			15	8	1	5	1			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	2	Total	Na	0	0
			2	2		

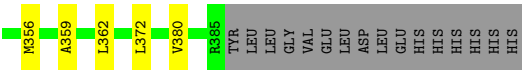
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		

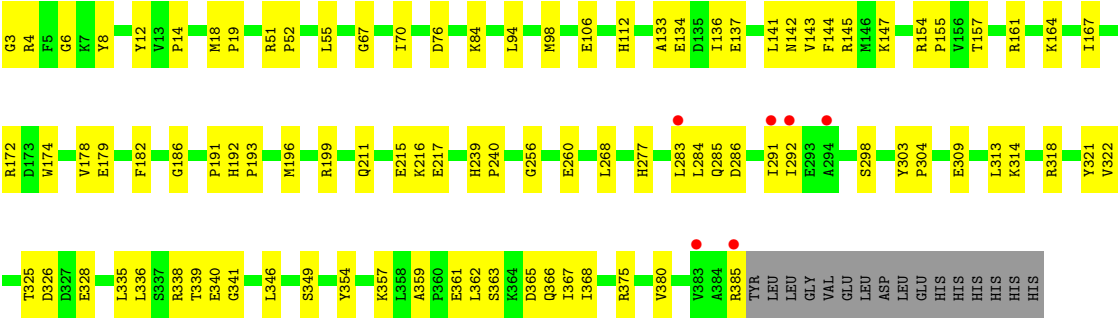
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	139	Total 139	O 139	0	0
6	C	44	Total 44	O 44	0	0
6	D	124	Total 124	O 124	0	0



• Molecule 2: LBCA-b



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.96Å 163.00Å 78.06Å 90.00° 93.78° 90.00°	Depositor
Resolution (Å)	47.26 – 1.97 47.26 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.26-1.97) 96.6 (47.26-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.178 , 0.232 0.183 , 0.231	Depositor DCC
R_{free} test set	4057 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9975	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: PLP, NA, G3P

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	0.41	0/1950	0.60	2/2653 (0.1%)
1	C	0.31	0/1791	0.50	1/2444 (0.0%)
2	B	0.34	1/2969 (0.0%)	0.53	0/4016
2	D	0.32	0/2968	0.51	0/4016
All	All	0.34	1/9678 (0.0%)	0.54	3/13129 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	84	LYS	C-O	-5.09	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	HIS	N-CA-C	-6.30	105.17	112.92
1	C	205	ASP	N-CA-C	5.74	119.47	112.23
1	A	107	PHE	N-CA-C	-5.18	103.64	110.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	LYS	Peptide
1	A	243	ASN	Peptide

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	1920	0	1893	65	0
1	C	1765	0	1722	83	0
2	B	2916	0	2883	50	0
2	D	2915	0	2877	81	0
3	A	10	0	7	0	0
3	C	10	0	7	1	0
4	B	15	8	7	0	0
4	D	15	0	7	3	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
6	A	91	0	0	3	1
6	B	139	0	0	6	1
6	C	44	0	0	7	0
6	D	124	0	0	9	1
All	All	9967	8	9403	263	2

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 14.

All (263) 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:D:84:LYS:HZ1	4:D:501:PLP:C4A	1.44	1.30
1:A:164:LYS:CD	1:A:203:HIS:ND1	2.08	1.17
2:D:84:LYS:NZ	4:D:501:PLP:C4A	2.05	1.17
1:C:247:GLU:HA	1:C:249:ILE:H	1.20	1.05
1:C:247:GLU:HA	1:C:249:ILE:N	1.76	0.99
1:C:79:ASP:OD2	6:C:401:HOH:O	1.82	0.98
1:C:171:SER:OG	6:C:402:HOH:O	1.85	0.94
1:A:37:VAL:HG11	1:A:88:LEU:HD11	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:HG22	1:C:205:ASP:H	1.34	0.91
1:A:201:ARG:HA	6:A:403:HOH:O	1.70	0.90
2:D:94:LEU:HG	2:D:98:MET:CE	2.02	0.90
1:A:243:ASN:C	1:A:245:ASP:HA	2.00	0.87
2:B:33:ASN:O	6:B:601:HOH:O	1.95	0.84
2:D:134:GLU:OE1	6:D:601:HOH:O	1.94	0.83
2:D:363:SER:OG	2:D:365:ASP:OD1	1.94	0.83
1:C:60:ASP:O	2:D:172:ARG:NH1	2.11	0.83
1:C:2:ASN:N	6:C:406:HOH:O	2.13	0.81
2:D:94:LEU:HG	2:D:98:MET:HE3	1.62	0.81
2:B:331:GLU:OE2	2:B:356:MET:HE1	1.80	0.81
1:A:187:SER:HA	1:A:219:GLN:HE22	1.46	0.81
1:C:199:ARG:HA	1:C:200:ILE:C	2.06	0.80
2:D:4:ARG:HD3	2:D:8:TYR:O	1.83	0.79
1:A:185:ALA:HB1	1:A:215:SER:HB3	1.64	0.79
2:B:28:TYR:CE2	2:B:32:LYS:HD2	2.18	0.78
2:D:260:GLU:OE1	2:D:260:GLU:N	2.18	0.77
2:D:55:LEU:O	2:D:216:LYS:HE3	1.84	0.76
2:D:3:GLY:N	6:D:604:HOH:O	2.17	0.76
1:C:6:GLU:OE2	6:C:404:HOH:O	2.03	0.76
1:C:61:GLY:N	1:C:182:VAL:CG1	2.49	0.76
1:C:237:VAL:HA	1:C:240:ILE:HD12	1.68	0.76
1:C:7:ALA:O	1:C:11:LEU:HD23	1.86	0.75
1:C:56:ASP:OD1	2:D:164:LYS:HG2	1.88	0.74
2:B:4:ARG:HD3	2:B:8:TYR:O	1.88	0.73
2:D:84:LYS:HZ2	4:D:501:PLP:C4A	2.01	0.73
2:D:385:ARG:O	6:D:602:HOH:O	2.07	0.72
1:A:107:PHE:O	1:A:108:ARG:HB3	1.90	0.72
2:D:325:THR:HG23	2:D:328:GLU:OE2	1.91	0.71
1:C:253:VAL:O	1:C:257:VAL:HG23	1.91	0.70
1:C:34:LEU:HD12	1:C:84:MET:HG2	1.72	0.69
1:A:1:MET:HG3	1:A:6:GLU:CG	2.23	0.69
2:B:4:ARG:HG3	2:B:6:GLY:O	1.92	0.69
1:A:199:ARG:HA	1:A:200:ILE:CB	2.23	0.68
2:B:18:MET:O	2:B:22:GLU:HG2	1.93	0.68
2:D:94:LEU:HG	2:D:98:MET:HE2	1.74	0.68
2:B:55:LEU:O	2:B:216:LYS:HE2	1.94	0.68
2:D:339:THR:HG23	2:D:340:GLU:HG2	1.75	0.68
2:B:328:GLU:O	2:B:331:GLU:HG3	1.94	0.67
1:A:107:PHE:O	1:A:108:ARG:CB	2.43	0.67
2:B:141:LEU:HD21	6:B:633:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:HB2	6:B:672:HOH:O	1.95	0.66
1:A:241:GLU:OE1	6:A:401:HOH:O	2.13	0.66
2:D:4:ARG:HG3	2:D:6:GLY:O	1.96	0.66
2:D:142:ASN:OD1	2:D:145:ARG:NH2	2.30	0.65
2:D:239:HIS:HB3	2:D:240:PRO:HD3	1.79	0.65
1:C:134:GLU:O	6:C:405:HOH:O	2.13	0.65
1:C:214:ILE:CD1	1:C:219:GLN:HB2	2.28	0.64
2:D:98:MET:HE1	2:D:182:PHE:HE1	1.63	0.64
2:B:268:LEU:O	2:B:314:LYS:HE3	1.97	0.63
1:A:246:GLU:O	1:A:248:ASP:N	2.31	0.63
2:B:136:ILE:CD1	2:B:155:PRO:HB3	2.29	0.63
1:C:60:ASP:C	1:C:182:VAL:CG1	2.72	0.63
1:A:135:GLU:OE1	2:B:4:ARG:NH2	2.32	0.62
1:C:118:CYS:HA	1:C:123:VAL:CG1	2.30	0.62
1:A:244:GLN:N	1:A:245:ASP:HA	2.14	0.62
1:A:187:SER:HA	1:A:219:GLN:NE2	2.14	0.62
2:B:261:THR:O	2:B:263:LYS:HD2	1.98	0.62
2:D:133:ALA:HB2	2:D:157:THR:HG22	1.82	0.62
2:B:91:GLN:OE1	2:B:184:ILE:HA	1.99	0.62
2:B:96:LYS:HG2	2:B:125:LEU:HD21	1.81	0.62
2:D:283:LEU:HD22	2:D:285:GLN:HB3	1.82	0.62
1:A:211:GLY:O	1:A:212:PHE:HB2	1.98	0.62
2:B:32:LYS:NZ	2:B:32:LYS:HB3	2.15	0.61
2:B:380:VAL:CG1	2:D:144:PHE:HD1	2.13	0.61
2:D:106:GLU:HG3	2:D:167:ILE:HG12	1.82	0.61
2:D:196:MET:HG3	2:D:199:ARG:NH2	2.15	0.61
2:B:144:PHE:CD2	2:D:380:VAL:HG13	2.36	0.60
2:D:239:HIS:ND1	6:D:608:HOH:O	2.31	0.60
1:C:204:THR:HG22	1:C:205:ASP:N	2.07	0.60
1:C:157:THR:HG23	2:D:19:PRO:HG2	1.83	0.60
1:A:1:MET:HG3	1:A:6:GLU:HG2	1.82	0.60
1:A:202:LYS:H	1:A:202:LYS:CD	2.15	0.60
2:B:7:LYS:HE2	2:B:8:TYR:CZ	2.36	0.60
1:C:29:ASP:OD1	1:C:31:GLU:HG3	2.01	0.59
2:D:362:LEU:HD12	2:D:368:ILE:HD11	1.84	0.59
2:B:199:ARG:HD3	2:B:309:GLU:OE1	2.03	0.59
2:B:239:HIS:HB3	2:B:240:PRO:HD3	1.85	0.59
2:D:211:GLN:O	2:D:215:GLU:HG3	2.03	0.58
1:A:150:LEU:HD22	1:A:152:PHE:CE1	2.38	0.58
1:C:131:LEU:O	6:C:407:HOH:O	2.17	0.58
2:D:286:ASP:HB3	2:D:292:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:VAL:O	1:C:226:VAL:HG22	2.04	0.58
2:D:283:LEU:CD2	2:D:285:GLN:HB3	2.34	0.58
2:D:363:SER:HB3	2:D:366:GLN:HG3	1.85	0.58
1:A:104:ASN:O	1:A:107:PHE:O	2.22	0.57
2:B:136:ILE:HD12	2:B:155:PRO:HB3	1.87	0.57
1:A:82:PHE:CD2	1:A:117:GLU:HG2	2.40	0.57
1:C:204:THR:CG2	1:C:205:ASP:H	2.10	0.56
2:D:375:ARG:NH1	6:D:607:HOH:O	2.25	0.56
1:C:244:GLN:O	1:C:246:GLU:N	2.39	0.56
1:C:101:THR:HG21	1:C:106:ILE:HD11	1.88	0.56
1:C:153:LEU:HG	1:C:175:TYR:HB3	1.87	0.56
2:D:336:LEU:HA	2:D:339:THR:HG22	1.88	0.56
2:D:309:GLU:O	2:D:313:LEU:HG	2.06	0.55
2:B:133:ALA:O	2:B:137:GLU:HG3	2.06	0.55
1:A:246:GLU:C	1:A:248:ASP:N	2.63	0.55
1:C:60:ASP:C	1:C:182:VAL:HG13	2.32	0.55
2:D:67:GLY:O	6:D:605:HOH:O	2.18	0.55
1:C:135:GLU:HG2	2:D:12:TYR:CZ	2.43	0.54
1:A:82:PHE:CE2	1:A:117:GLU:HG2	2.43	0.54
2:B:47:ASP:OD2	2:D:216:LYS:NZ	2.29	0.54
2:B:380:VAL:HG13	2:D:144:PHE:CD1	2.42	0.54
1:C:156:PRO:HD3	1:C:177:VAL:O	2.07	0.54
2:D:318:ARG:HA	6:D:613:HOH:O	2.08	0.54
1:C:233:GLY:HA3	3:C:301:G3P:H2	1.90	0.54
1:A:243:ASN:O	1:A:245:ASP:HA	2.07	0.53
2:D:303:TYR:CD1	2:D:304:PRO:HD2	2.44	0.53
1:C:35:GLU:OE2	1:C:38:ARG:NH1	2.41	0.53
2:D:112:HIS:CE1	2:D:186:GLY:HA2	2.43	0.53
1:C:132:PRO:HG3	2:D:18:MET:CE	2.38	0.53
2:D:164:LYS:HD2	2:D:291:ILE:HB	1.91	0.53
1:A:244:GLN:N	1:A:245:ASP:CA	2.71	0.53
1:A:182:VAL:HG12	6:A:460:HOH:O	2.09	0.53
2:D:154:ARG:HG2	2:D:154:ARG:HH11	1.73	0.53
2:D:335:LEU:O	2:D:339:THR:HG22	2.09	0.53
1:A:1:MET:CG	1:A:6:GLU:HG2	2.39	0.53
1:C:247:GLU:CA	1:C:249:ILE:H	2.07	0.53
2:B:335:LEU:O	2:B:339:THR:HG23	2.09	0.52
1:A:240:ILE:HA	1:A:249:ILE:HG23	1.90	0.52
1:A:246:GLU:C	1:A:248:ASP:H	2.17	0.52
1:A:199:ARG:CA	1:A:200:ILE:CB	2.88	0.52
1:A:234:SER:O	1:A:238:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HD12	1:C:84:MET:CG	2.39	0.51
2:D:328:GLU:OE2	6:D:606:HOH:O	2.19	0.51
1:C:6:GLU:O	1:C:10:GLU:HG2	2.09	0.51
1:A:218:GLU:O	1:A:222:GLU:HG3	2.10	0.51
1:A:202:LYS:CD	1:A:202:LYS:N	2.73	0.51
1:A:60:ASP:C	1:A:182:VAL:HG22	2.36	0.51
1:C:204:THR:CG2	1:C:205:ASP:N	2.73	0.51
1:C:182:VAL:CG1	1:C:183:THR:N	2.73	0.51
2:B:380:VAL:CG1	2:D:144:PHE:CD1	2.94	0.51
1:C:34:LEU:HD21	1:C:38:ARG:NH2	2.25	0.51
2:B:144:PHE:HD2	2:D:380:VAL:HG13	1.76	0.51
1:A:143:ALA:HB1	1:A:148:VAL:O	2.11	0.51
2:D:286:ASP:HB3	2:D:292:ILE:CD1	2.41	0.50
2:D:338:ARG:NH2	6:D:603:HOH:O	2.13	0.50
1:A:37:VAL:HG13	1:A:48:ILE:HD13	1.93	0.50
1:C:118:CYS:CA	1:C:123:VAL:CG1	2.89	0.50
2:D:106:GLU:HG3	2:D:167:ILE:CG1	2.41	0.50
1:C:118:CYS:HB3	1:C:123:VAL:HG13	1.94	0.50
1:C:153:LEU:HD23	1:C:177:VAL:CG2	2.42	0.50
1:C:115:VAL:HG11	1:C:143:ALA:HA	1.93	0.50
2:D:134:GLU:O	2:D:137:GLU:HG2	2.11	0.49
1:A:133:PRO:HB2	1:A:165:MET:SD	2.52	0.49
1:C:214:ILE:HD11	1:C:220:ALA:N	2.27	0.49
1:C:61:GLY:CA	1:C:182:VAL:CG1	2.90	0.49
2:B:145:ARG:HD3	6:B:633:HOH:O	2.12	0.49
1:C:101:THR:O	1:C:128:VAL:HA	2.12	0.49
2:D:157:THR:HA	2:D:161:ARG:HG2	1.94	0.49
1:C:243:ASN:O	1:C:245:ASP:N	2.46	0.49
2:D:143:VAL:HG12	2:D:147:LYS:HE3	1.95	0.49
1:C:214:ILE:HD13	1:C:219:GLN:CB	2.43	0.49
1:A:83:GLU:O	1:A:87:GLU:HG2	2.12	0.49
1:A:167:ALA:HB1	1:A:204:THR:HB	1.95	0.48
2:D:154:ARG:HG2	2:D:154:ARG:NH1	2.28	0.48
1:C:157:THR:CG2	2:D:19:PRO:HG2	2.43	0.48
1:A:145:LYS:HD3	1:A:146:TYR:CE1	2.48	0.48
1:A:61:GLY:HA3	1:A:183:THR:O	2.13	0.48
1:C:199:ARG:CA	1:C:200:ILE:C	2.84	0.48
2:B:59:GLU:HG2	2:B:63:LYS:HE2	1.95	0.48
1:C:223:VAL:CG1	1:C:230:VAL:HG12	2.44	0.48
2:D:179:GLU:CD	2:D:179:GLU:H	2.21	0.48
1:A:1:MET:SD	1:A:6:GLU:HG2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:GLU:OE1	2:D:357:LYS:NZ	2.39	0.47
1:C:99:PHE:HB2	1:C:126:LEU:HD23	1.96	0.47
1:C:115:VAL:O	1:C:118:CYS:HB2	2.15	0.47
1:C:247:GLU:N	1:C:248:ASP:CB	2.77	0.47
1:A:116:LYS:O	1:A:120:GLU:HG3	2.14	0.47
1:A:59:ALA:C	1:A:182:VAL:HG23	2.40	0.47
2:B:342:ILE:HG21	2:B:372:LEU:HD21	1.97	0.47
1:C:151:ILE:N	1:C:151:ILE:HD12	2.30	0.46
1:C:214:ILE:HD12	1:C:215:SER:N	2.31	0.46
1:C:37:VAL:O	1:C:41:VAL:HG23	2.16	0.46
1:A:109:TYR:CE2	1:A:113:ARG:HG2	2.51	0.46
1:A:165:MET:HE3	1:A:165:MET:HB3	1.68	0.46
2:D:98:MET:CE	2:D:182:PHE:HE1	2.27	0.46
2:D:314:LYS:HB2	2:D:321:TYR:CD2	2.51	0.46
1:C:3:ARG:HB3	1:C:96:PRO:HB3	1.97	0.46
1:C:61:GLY:N	1:C:182:VAL:HG12	2.31	0.45
1:C:118:CYS:CB	1:C:123:VAL:HG13	2.46	0.45
1:C:38:ARG:NE	6:C:403:HOH:O	1.90	0.45
1:C:251:GLU:OE2	1:C:251:GLU:HA	2.15	0.45
2:D:217:GLU:HG3	2:D:367:ILE:HD13	1.98	0.45
2:D:70:ILE:HD11	2:D:359:ALA:HB2	1.98	0.45
2:D:174:TRP:O	2:D:178:VAL:HG22	2.16	0.45
1:C:165:MET:HE3	1:C:165:MET:HB3	1.75	0.45
2:B:112:HIS:CE1	2:B:186:GLY:HA2	2.52	0.44
1:C:57:PRO:HB2	1:C:60:ASP:HB2	1.99	0.44
2:D:322:VAL:HG21	2:D:354:TYR:CE2	2.52	0.44
2:D:192:HIS:ND1	2:D:193:PRO:HA	2.32	0.44
2:B:70:ILE:HD11	2:B:359:ALA:HB2	1.99	0.44
1:C:16:GLU:OE2	1:C:16:GLU:HA	2.18	0.44
1:A:95:VAL:HG13	1:A:95:VAL:O	2.17	0.44
1:C:61:GLY:CA	1:C:182:VAL:HG12	2.47	0.44
1:A:1:MET:HG3	1:A:6:GLU:HG3	1.96	0.44
1:A:115:VAL:HG11	1:A:143:ALA:HA	2.00	0.44
1:A:60:ASP:C	1:A:182:VAL:CG2	2.90	0.44
1:A:185:ALA:HB1	1:A:215:SER:CB	2.42	0.43
2:B:239:HIS:HA	2:B:242:ILE:HG12	2.00	0.43
1:C:58:LEU:HD23	2:D:14:PRO:HD3	1.99	0.43
2:B:7:LYS:HE2	2:B:8:TYR:OH	2.18	0.43
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.75	0.43
1:C:50:LEU:HD13	1:C:84:MET:HE1	2.00	0.43
2:D:256:GLY:HA2	2:D:326:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ALA:HB2	2:B:362:LEU:HB2	2.01	0.43
2:D:268:LEU:HD13	2:D:321:TYR:CG	2.54	0.43
2:D:365:ASP:OD1	2:D:365:ASP:N	2.47	0.43
1:A:58:LEU:HD23	2:B:14:PRO:HD3	2.00	0.43
1:C:244:GLN:C	1:C:246:GLU:H	2.26	0.43
1:C:223:VAL:HG12	1:C:230:VAL:HG12	2.00	0.43
2:D:191:PRO:HD3	2:D:277:HIS:O	2.19	0.43
2:B:160:SER:OG	2:B:165:ASP:OD1	2.27	0.43
1:C:174:VAL:CG2	1:C:208:ILE:HG12	2.48	0.42
2:B:96:LYS:HD2	2:B:123:PHE:HB3	2.01	0.42
2:D:76:ASP:HB2	2:D:375:ARG:HB3	2.02	0.42
1:C:145:LYS:HE3	1:C:146:TYR:CE2	2.54	0.42
2:D:283:LEU:HD23	2:D:284:LEU:C	2.44	0.42
1:A:22:PHE:CD2	1:A:22:PHE:C	2.97	0.42
2:B:286:ASP:HB3	2:B:292:ILE:HD11	2.01	0.42
2:B:268:LEU:HD13	2:B:321:TYR:CD1	2.55	0.42
2:B:265:ALA:CB	2:B:294:ALA:HB1	2.49	0.42
1:A:30:LEU:CD1	1:A:80:LYS:HB3	2.49	0.42
2:B:106:GLU:HG3	2:B:167:ILE:CG1	2.49	0.42
2:B:168:ASN:O	2:B:172:ARG:HG3	2.20	0.42
1:A:185:ALA:CB	1:A:215:SER:HB3	2.42	0.42
2:D:268:LEU:O	2:D:314:LYS:NZ	2.47	0.42
1:A:199:ARG:CB	1:A:201:ARG:HG3	2.50	0.42
1:C:11:LEU:HD12	1:C:16:GLU:CB	2.49	0.41
1:C:45:ALA:CB	1:C:48:ILE:HD11	2.50	0.41
1:A:160:ASP:O	1:A:164:LYS:HG2	2.20	0.41
1:A:184:GLY:O	1:A:213:GLY:HA2	2.21	0.41
2:B:149:LEU:HD22	2:D:341:GLY:HA2	2.02	0.41
1:A:108:ARG:HA	1:A:108:ARG:HD2	1.82	0.41
2:B:32:LYS:HB3	2:B:32:LYS:HZ3	1.84	0.41
1:C:60:ASP:C	1:C:182:VAL:HG11	2.44	0.41
2:B:28:TYR:CE2	2:B:32:LYS:CD	2.99	0.41
1:A:203:HIS:CD2	1:A:203:HIS:N	2.88	0.41
2:B:257:LYS:NZ	6:B:610:HOH:O	2.47	0.41
2:D:51:ARG:HB3	2:D:52:PRO:HA	2.03	0.41
2:D:136:ILE:HD12	2:D:155:PRO:HB3	2.03	0.41
2:D:283:LEU:HD23	2:D:284:LEU:N	2.36	0.41
1:C:175:TYR:HD2	1:C:175:TYR:C	2.29	0.41
1:A:106:ILE:C	1:A:107:PHE:O	2.64	0.40
1:A:125:GLY:O	1:A:126:LEU:HD23	2.22	0.40
2:B:145:ARG:CD	6:B:633:HOH:O	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:PHE:CD2	1:C:22:PHE:C	2.99	0.40
1:C:182:VAL:HG12	1:C:183:THR:N	2.36	0.40
1:C:247:GLU:H	1:C:248:ASP:CB	2.34	0.40
2:B:51:ARG:HB3	2:B:52:PRO:HA	2.03	0.40
1:A:2:ASN:O	1:A:6:GLU:HG3	2.21	0.40
1:C:178:SER:OG	1:C:212:PHE:O	2.39	0.40
1:C:200:ILE:O	1:C:201:ARG:CB	2.69	0.40
1:A:38:ARG:O	1:A:42:GLU:HG2	2.22	0.40
2:D:298:SER:HB3	2:D:346:LEU:HB3	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:632:HOH:O	6:D:632:HOH:O[2_556]	1.85	0.35
6:A:451:HOH:O	6:B:720:HOH:O[2_557]	2.11	0.09

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	257/273 (94%)	243 (95%)	8 (3%)	6 (2%)	5	1
1	C	241/273 (88%)	223 (92%)	13 (5%)	5 (2%)	5	1
2	B	381/399 (96%)	375 (98%)	6 (2%)	0	100	100
2	D	381/399 (96%)	372 (98%)	9 (2%)	0	100	100
All	All	1260/1344 (94%)	1213 (96%)	36 (3%)	11 (1%)	14	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLU
1	C	201	ARG
1	C	202	LYS
1	C	203	HIS
1	A	200	ILE
1	A	202	LYS
1	A	245	ASP
1	A	247	GLU
1	C	244	GLN
1	A	248	ASP
1	C	248	ASP

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	190/223 (85%)	186 (98%)	4 (2%)	47	40
1	C	171/223 (77%)	166 (97%)	5 (3%)	37	28
2	B	298/315 (95%)	295 (99%)	3 (1%)	68	65
2	D	298/315 (95%)	295 (99%)	3 (1%)	68	65
All	All	957/1076 (89%)	942 (98%)	15 (2%)	55	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	198	SER
1	A	203	HIS
1	A	215	SER
2	B	272	ARG
2	B	297	ILE
2	B	348	SER
1	C	4	ILE
1	C	31	GLU
1	C	35	GLU
1	C	123	VAL

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Mol	Chain	Res	Type
1	C	214	ILE
2	D	141	LEU
2	D	349	SER
2	D	361	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	33	ASN
2	D	168	ASN
2	D	334	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 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	$\# Z > 2$
3	G3P	A	301	-	9,9,9	0.95	0	10,12,12	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLP	B	501	2	15,15,16	1.51	3 (20%)	21,22,23	1.43	4 (19%)
3	G3P	C	301	-	9,9,9	0.92	0	10,12,12	0.61	0
4	PLP	D	501	-	15,15,16	1.97	5 (33%)	21,22,23	1.27	2 (9%)

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
3	G3P	A	301	-	-	3/8/8/8	-
4	PLP	B	501	2	-	0/6/6/8	0/1/1/1
3	G3P	C	301	-	-	4/8/8/8	-
4	PLP	D	501	-	-	0/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	PLP	C5-C4	-4.60	1.35	1.40
4	D	501	PLP	C3-C2	-3.28	1.37	1.41
4	B	501	PLP	C3-C2	-2.89	1.38	1.41
4	D	501	PLP	C3-C4	-2.66	1.35	1.40
4	B	501	PLP	C5-C4	-2.66	1.37	1.40
4	D	501	PLP	P-O3P	-2.30	1.46	1.54
4	D	501	PLP	P-O2P	-2.29	1.46	1.54
4	B	501	PLP	C3-C4	-2.23	1.35	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	PLP	C4A-C4-C3	-2.60	116.18	120.52
4	D	501	PLP	C4A-C4-C5	2.57	123.59	120.94
4	B	501	PLP	C4A-C4-C5	2.54	123.56	120.94
4	B	501	PLP	C5-C6-N1	-2.41	119.91	123.83
4	D	501	PLP	C2A-C2-N1	2.39	122.14	117.64
4	B	501	PLP	C2A-C2-N1	2.26	121.89	117.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	G3P	C1-C2-C3-O1P
3	C	301	G3P	O2-C2-C3-O1P
3	A	301	G3P	O2-C2-C3-O1P
3	A	301	G3P	C1-C2-C3-O1P
3	C	301	G3P	C2-C3-O1P-P
3	A	301	G3P	C2-C3-O1P-P
3	C	301	G3P	C3-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	G3P	1	0
4	D	501	PLP	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	261/273 (95%)	0.28	10 (3%) 44 54	27, 43, 71, 93	0
1	C	245/273 (89%)	0.58	20 (8%) 17 24	34, 56, 81, 95	0
2	B	383/399 (95%)	-0.07	0 100 100	23, 36, 61, 78	0
2	D	383/399 (95%)	0.12	6 (1%) 70 79	25, 42, 69, 94	0
All	All	1272/1344 (94%)	0.19	36 (2%) 55 65	23, 43, 72, 95	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	183	THR	4.4
1	A	200	ILE	4.1
1	A	180	THR	3.5
1	A	186	ARG	3.3
1	C	203	HIS	3.1
1	C	180	THR	3.1
1	C	246	GLU	3.1
1	A	266	LEU	3.0
1	C	212	PHE	2.9
1	A	248	ASP	2.8
1	C	249	ILE	2.8
1	C	244	GLN	2.7
1	C	58	LEU	2.7
1	C	182	VAL	2.7
1	C	204	THR	2.6
1	A	244	GLN	2.6
1	A	189	ILE	2.6
1	A	182	VAL	2.6
1	C	200	ILE	2.5
1	C	176	CYS	2.4
1	A	58	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	202	LYS	2.3
2	D	283	LEU	2.3
1	C	59	ALA	2.3
1	C	179	VAL	2.3
1	C	201	ARG	2.2
2	D	294	ALA	2.2
1	A	183	THR	2.2
1	C	199	ARG	2.2
2	D	291	ILE	2.2
2	D	292	ILE	2.1
1	C	247	GLU	2.1
2	D	383	VAL	2.1
2	D	385	ARG	2.1
1	C	181	GLY	2.1
1	C	245	ASP	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($\text{\AA}^2$)	Q<0.9
5	NA	D	502	1/1	0.90	0.14	61,61,61,61	0
3	G3P	C	301	10/10	0.91	0.10	54,70,78,79	0
5	NA	D	503	1/1	0.91	0.09	52,52,52,52	0
4	PLP	D	501	15/16	0.92	0.11	35,47,67,71	0
4	PLP	B	501	15/16	0.93	0.09	39,53,64,72	0
3	G3P	A	301	10/10	0.95	0.07	35,42,44,45	0
5	NA	B	502	1/1	0.96	0.16	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.