



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 PM UTC

PDB ID : 3MC6 / pdb_00003mc6
Title : Crystal structure of ScDPL1
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Deposited on : 2010-03-27
Resolution : 3.15 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

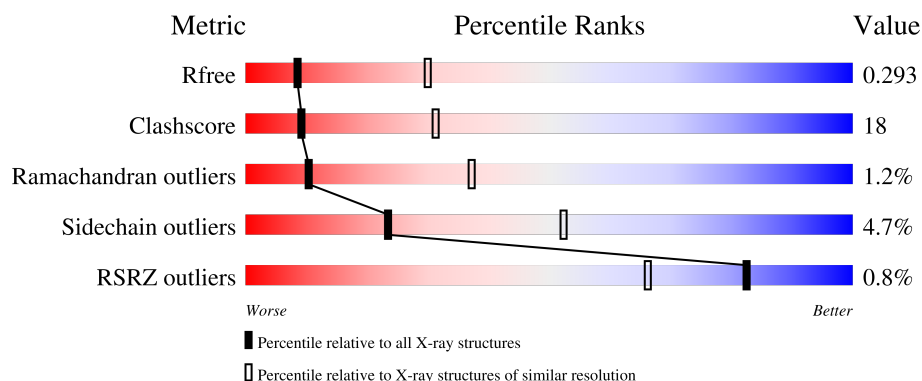
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	497	 52% 30% 14%
2	C	497	 53% 29% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6634 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 Sphingosine-1-phosphate lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	426	3320	2123	559	615	1	22	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MET	-	initiating methionine	UNP Q05567
A	102	GLY	-	expression tag	UNP Q05567
A	308	VAL	ILE	engineered mutation	UNP Q05567
A	469	ASP	ASN	engineered mutation	UNP Q05567
A	590	LEU	-	expression tag	UNP Q05567
A	591	GLU	-	expression tag	UNP Q05567
A	592	HIS	-	expression tag	UNP Q05567
A	593	HIS	-	expression tag	UNP Q05567
A	594	HIS	-	expression tag	UNP Q05567
A	595	HIS	-	expression tag	UNP Q05567
A	596	HIS	-	expression tag	UNP Q05567
A	597	HIS	-	expression tag	UNP Q05567

- Molecule 2 is a protein called Sphingosine-1-phosphate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	424	3295	2108	556	609	22	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

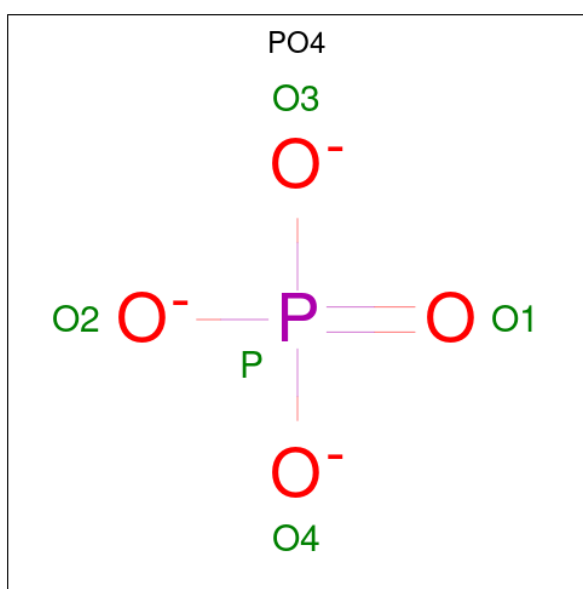
Chain	Residue	Modelled	Actual	Comment	Reference
C	101	MET	-	initiating methionine	UNP Q05567
C	102	GLY	-	expression tag	UNP Q05567
C	308	VAL	ILE	engineered mutation	UNP Q05567
C	469	ASP	ASN	engineered mutation	UNP Q05567

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Chain	Residue	Modelled	Actual	Comment	Reference
C	590	LEU	-	expression tag	UNP Q05567
C	591	GLU	-	expression tag	UNP Q05567
C	592	HIS	-	expression tag	UNP Q05567
C	593	HIS	-	expression tag	UNP Q05567
C	594	HIS	-	expression tag	UNP Q05567
C	595	HIS	-	expression tag	UNP Q05567
C	596	HIS	-	expression tag	UNP Q05567
C	597	HIS	-	expression tag	UNP Q05567

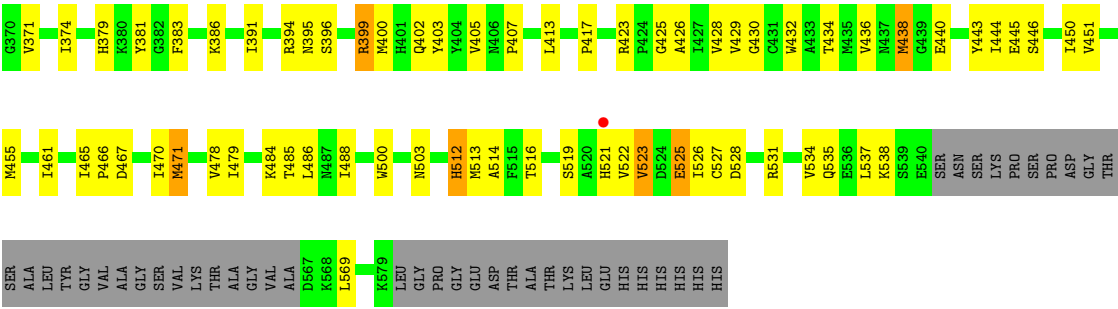
- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	151.10Å 156.86Å 201.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.92 – 3.15 41.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.92-3.15) 99.1 (41.92-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.241 , 0.300 0.240 , 0.293	Depositor DCC
R_{free} test set	610 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 128.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6634	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: PO4, LLP

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	0.26	0/3373	0.72	1/4570 (0.0%)
2	C	0.26	0/3373	0.72	3/4570 (0.1%)
All	All	0.26	0/6746	0.72	4/9140 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ASP	N-CA-C	5.39	115.15	108.19
2	C	365	ASP	N-CA-C	5.36	115.11	108.19
2	C	159	ILE	CA-C-N	5.09	125.37	119.92
2	C	159	ILE	C-N-CA	5.09	125.37	119.92

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3304	125	0
2	C	3295	0	3288	120	0
3	A	5	0	0	0	0
3	C	10	0	0	0	0
4	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
All	All	6634	0	6592	241	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 18.

All (241) 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:230:THR:HG23	1:A:391:ILE:HG23	1.64	0.78
2:C:230:THR:HG23	2:C:391:ILE:HG23	1.64	0.77
1:A:262:ILE:HG22	1:A:283:ARG:HB2	1.68	0.75
2:C:262:ILE:HG22	2:C:283:ARG:HB2	1.67	0.74
1:A:257:THR:HG23	1:A:258:GLU:HG2	1.72	0.72
2:C:257:THR:HG23	2:C:258:GLU:HG2	1.72	0.72
1:A:170:SER:HB2	1:A:514:ALA:H	1.58	0.68
2:C:170:SER:HB2	2:C:514:ALA:H	1.59	0.68
1:A:324:ASP:O	1:A:328:LEU:HB2	1.94	0.67
2:C:324:ASP:O	2:C:328:LEU:HB2	1.94	0.67
1:A:461:ILE:HG22	1:A:465:ILE:HD12	1.77	0.66
2:C:461:ILE:HG22	2:C:465:ILE:HD12	1.77	0.66
2:C:247:LYS:O	2:C:251:LEU:HB2	1.96	0.65
1:A:247:LYS:O	1:A:251:LEU:HB2	1.97	0.65
2:C:206:ARG:HD3	2:C:206:ARG:C	2.24	0.63
2:C:296:LEU:HD12	2:C:296:LEU:H	1.64	0.63
1:A:206:ARG:HD3	1:A:206:ARG:C	2.24	0.62
2:C:211:GLU:O	2:C:215:MET:HG3	1.99	0.62
1:A:211:GLU:O	1:A:215:MET:HG3	1.99	0.62
1:A:296:LEU:H	1:A:296:LEU:HD12	1.64	0.62
2:C:216:VAL:HA	2:C:219:MET:HE2	1.81	0.62
2:C:291:THR:HG23	2:C:293:GLN:H	1.65	0.62
1:A:216:VAL:HA	1:A:219:MET:HE2	1.81	0.61
2:C:485:THR:HB	2:C:486:LEU:HD22	1.82	0.61
1:A:291:THR:HG23	1:A:293:GLN:H	1.65	0.61
1:A:485:THR:HB	1:A:486:LEU:HD22	1.82	0.61
2:C:379:HIS:HB2	2:C:386:LYS:HA	1.82	0.61
1:A:146:ASP:O	1:A:149:ILE:HD13	2.01	0.61
1:A:287:LEU:HB3	1:A:293:GLN:O	2.01	0.61
1:A:379:HIS:HB2	1:A:386:LYS:HA	1.82	0.60
2:C:403:TYR:HD1	2:C:417:PRO:HA	1.65	0.60
1:A:329:GLY:HA3	1:A:368:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:PRO:HG2	2:C:394:ARG:HG3	1.83	0.60
2:C:287:LEU:HB3	2:C:293:GLN:O	2.02	0.60
1:A:403:TYR:HD1	1:A:417:PRO:HA	1.66	0.60
2:C:146:ASP:O	2:C:149:ILE:HD13	2.01	0.60
2:C:329:GLY:HA3	2:C:368:VAL:HG12	1.83	0.60
2:C:443:TYR:HA	2:C:446:SER:HB3	1.84	0.59
1:A:438:MET:HA	1:A:438:MET:HE2	1.83	0.59
1:A:443:TYR:HA	1:A:446:SER:HB3	1.83	0.59
2:C:438:MET:HA	2:C:438:MET:HE2	1.83	0.59
2:C:347:SER:OG	2:C:381:TYR:HB2	2.04	0.58
1:A:283:ARG:HB3	1:A:283:ARG:NH1	2.19	0.58
2:C:283:ARG:NH1	2:C:283:ARG:HB3	2.19	0.58
1:A:223:PRO:HG2	1:A:394:ARG:HG3	1.84	0.58
1:A:503:ASN:HB2	1:A:512:HIS:CE1	2.39	0.58
1:A:347:SER:OG	1:A:381:TYR:HB2	2.04	0.57
1:A:265:VAL:HG12	1:A:284:HIS:HB3	1.86	0.57
2:C:265:VAL:HG12	2:C:284:HIS:HB3	1.86	0.57
2:C:503:ASN:HB2	2:C:512:HIS:CE1	2.39	0.57
2:C:180:LEU:HD21	2:C:434:THR:HG22	1.86	0.57
1:A:180:LEU:HD21	1:A:434:THR:HG22	1.85	0.57
2:C:425:GLY:O	2:C:428:VAL:HG22	2.06	0.55
1:A:368:VAL:HB	1:A:371:VAL:HG23	1.88	0.55
1:A:527:CYS:O	1:A:531:ARG:HG3	2.07	0.55
1:A:371:VAL:HG11	1:A:374:ILE:HD11	1.89	0.54
2:C:527:CYS:O	2:C:531:ARG:HG3	2.07	0.54
2:C:300:LYS:HA	2:C:303:ILE:HD13	1.89	0.54
2:C:310:LEU:HD23	2:C:338:PRO:O	2.07	0.54
2:C:368:VAL:HB	2:C:371:VAL:HG23	1.88	0.54
2:C:371:VAL:HG11	2:C:374:ILE:HD11	1.88	0.54
1:A:500:TRP:CZ3	1:A:525:GLU:HB3	2.43	0.54
1:A:380:LLP:HE3	4:A:3:HOH:O	2.08	0.54
1:A:425:GLY:O	1:A:428:VAL:HG22	2.07	0.54
2:C:500:TRP:CZ3	2:C:525:GLU:HB3	2.43	0.54
1:A:310:LEU:HD23	1:A:338:PRO:O	2.08	0.53
2:C:534:VAL:HG13	2:C:538:LYS:NZ	2.23	0.53
1:A:300:LYS:HA	1:A:303:ILE:HD13	1.89	0.53
1:A:329:GLY:HA3	1:A:368:VAL:CG1	2.38	0.53
2:C:329:GLY:HA3	2:C:368:VAL:CG1	2.37	0.53
2:C:461:ILE:HD11	2:C:470:ILE:HD11	1.91	0.53
1:A:377:ASP:OD2	1:A:380:LLP:HE2	2.09	0.52
1:A:534:VAL:HG13	1:A:538:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HD12	1:A:371:VAL:HG22	1.91	0.52
2:C:339:LEU:HD12	2:C:371:VAL:HG22	1.91	0.52
1:A:461:ILE:HD11	1:A:470:ILE:HD11	1.92	0.52
2:C:272:ASP:HA	2:C:282:LEU:HD22	1.91	0.52
2:C:430:GLY:O	2:C:434:THR:HG23	2.09	0.52
1:A:259:PRO:HB2	1:A:280:MET:HG2	1.92	0.52
1:A:272:ASP:HA	1:A:282:LEU:HD22	1.91	0.52
1:A:525:GLU:HA	1:A:528:ASP:HB3	1.93	0.51
2:C:177:GLY:O	2:C:181:ILE:HD13	2.10	0.51
2:C:405:VAL:HG12	2:C:407:PRO:HD3	1.91	0.51
1:A:405:VAL:HG12	1:A:407:PRO:HD3	1.91	0.51
2:C:259:PRO:HB2	2:C:280:MET:HG2	1.92	0.51
2:C:525:GLU:HA	2:C:528:ASP:HB3	1.93	0.51
1:A:430:GLY:O	1:A:434:THR:HG23	2.10	0.51
1:A:170:SER:HB3	1:A:513:MET:SD	2.51	0.50
1:A:177:GLY:O	1:A:181:ILE:HD13	2.11	0.50
1:A:178:ASP:CG	2:C:531:ARG:HG2	2.37	0.50
1:A:333:GLN:OE1	1:A:369:PRO:HB2	2.12	0.50
2:C:170:SER:HB3	2:C:513:MET:SD	2.52	0.50
1:A:310:LEU:HG	1:A:339:LEU:HD23	1.94	0.50
1:A:569:LEU:O	1:A:569:LEU:HD23	2.11	0.50
2:C:310:LEU:HG	2:C:339:LEU:HD23	1.94	0.50
2:C:207:LYS:HE3	2:C:211:GLU:OE2	2.12	0.49
1:A:399:ARG:O	1:A:402:GLN:HG2	2.13	0.49
2:C:399:ARG:O	2:C:402:GLN:HG2	2.12	0.49
1:A:207:LYS:HE3	1:A:211:GLU:OE2	2.13	0.49
2:C:333:GLN:OE1	2:C:369:PRO:HB2	2.12	0.49
2:C:365:ASP:OD1	2:C:367:ARG:HD3	2.13	0.49
2:C:403:TYR:CD1	2:C:417:PRO:HA	2.46	0.49
2:C:365:ASP:CG	2:C:367:ARG:HD3	2.38	0.49
1:A:365:ASP:OD1	1:A:367:ARG:HD3	2.13	0.48
1:A:403:TYR:CD1	1:A:417:PRO:HA	2.46	0.48
2:C:569:LEU:O	2:C:569:LEU:HD23	2.12	0.48
1:A:175:HIS:HB2	1:A:383:PHE:CD2	2.49	0.48
2:C:154:LYS:O	2:C:158:LEU:HB2	2.14	0.48
2:C:537:LEU:HD12	2:C:538:LYS:HG3	1.96	0.48
1:A:235:GLY:O	1:A:239:LEU:HD13	2.14	0.48
1:A:365:ASP:CG	1:A:367:ARG:HD3	2.38	0.48
2:C:175:HIS:HB2	2:C:383:PHE:CD2	2.49	0.48
2:C:310:LEU:HD23	2:C:310:LEU:H	1.78	0.48
2:C:432:TRP:O	2:C:436:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LEU:HD12	1:A:538:LYS:HG3	1.96	0.48
1:A:516:THR:H	1:A:519:SER:HG	1.61	0.47
2:C:235:GLY:O	2:C:239:LEU:HD13	2.14	0.47
2:C:512:HIS:ND1	2:C:512:HIS:C	2.73	0.47
1:A:432:TRP:O	1:A:436:VAL:HG23	2.14	0.47
1:A:154:LYS:O	1:A:158:LEU:HB2	2.14	0.47
1:A:310:LEU:HD23	1:A:310:LEU:H	1.78	0.47
1:A:226:THR:O	1:A:395:ASN:HA	2.15	0.47
1:A:512:HIS:ND1	1:A:512:HIS:C	2.73	0.46
2:C:226:THR:O	2:C:395:ASN:HA	2.16	0.46
1:A:531:ARG:O	1:A:535:GLN:HG3	2.16	0.46
2:C:516:THR:H	2:C:519:SER:HG	1.62	0.46
2:C:396:SER:HA	2:C:399:ARG:HD2	1.97	0.46
2:C:186:ILE:O	2:C:190:LYS:HG2	2.16	0.46
2:C:230:THR:HG21	2:C:402:GLN:NE2	2.31	0.46
2:C:467:ASP:HB3	2:C:486:LEU:HD21	1.98	0.46
1:A:186:ILE:O	1:A:190:LYS:HG2	2.16	0.46
2:C:523:VAL:HA	2:C:526:ILE:HD11	1.98	0.46
2:C:531:ARG:O	2:C:535:GLN:HG3	2.16	0.46
1:A:223:PRO:C	1:A:225:ASP:H	2.24	0.45
2:C:366:PHE:CE2	2:C:374:ILE:HD12	2.50	0.45
1:A:366:PHE:CE2	1:A:374:ILE:HD12	2.51	0.45
2:C:349:ILE:O	2:C:353:MET:HG2	2.16	0.45
1:A:230:THR:HG21	1:A:402:GLN:NE2	2.31	0.45
1:A:467:ASP:HB3	1:A:486:LEU:HD21	1.98	0.45
2:C:208:MET:O	2:C:212:VAL:HG23	2.16	0.45
1:A:181:ILE:HA	1:A:184:GLN:HE21	1.81	0.45
1:A:413:LEU:N	1:A:413:LEU:HD23	2.32	0.45
2:C:181:ILE:HA	2:C:184:GLN:HE21	1.82	0.45
2:C:186:ILE:HD12	2:C:186:ILE:C	2.42	0.45
2:C:451:VAL:O	2:C:455:MET:HG2	2.17	0.45
2:C:194:ALA:HB1	2:C:205:VAL:HG21	1.99	0.45
1:A:132:LEU:HD12	1:A:132:LEU:O	2.17	0.45
1:A:281:LYS:HE3	1:A:283:ARG:HD2	1.99	0.45
1:A:149:ILE:HA	1:A:152:LEU:HD12	1.98	0.44
1:A:349:ILE:O	1:A:353:MET:HG2	2.16	0.44
1:A:208:MET:O	1:A:212:VAL:HG23	2.17	0.44
2:C:132:LEU:HD12	2:C:132:LEU:O	2.17	0.44
2:C:223:PRO:C	2:C:225:ASP:H	2.24	0.44
2:C:317:PHE:N	2:C:318:PRO:CD	2.80	0.44
1:A:523:VAL:HA	1:A:526:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ILE:HA	2:C:152:LEU:HD12	1.99	0.44
1:A:396:SER:HA	1:A:399:ARG:HD2	1.98	0.44
1:A:531:ARG:HG2	2:C:178:ASP:CG	2.42	0.44
2:C:281:LYS:HE3	2:C:283:ARG:HD2	2.00	0.44
1:A:186:ILE:HD12	1:A:186:ILE:C	2.42	0.44
2:C:400:MET:HA	2:C:403:TYR:CD2	2.52	0.44
1:A:132:LEU:HD22	1:A:155:LEU:HD23	2.00	0.44
1:A:144:PRO:O	1:A:148:VAL:HG23	2.18	0.44
1:A:228:CYS:SG	1:A:399:ARG:HG2	2.58	0.44
2:C:328:LEU:HD12	2:C:331:ILE:HG21	2.00	0.44
2:C:413:LEU:HD23	2:C:413:LEU:N	2.32	0.44
1:A:465:ILE:N	1:A:466:PRO:HD3	2.33	0.43
2:C:522:VAL:HG22	2:C:526:ILE:HG23	2.00	0.43
1:A:194:ALA:HB1	1:A:205:VAL:HG21	1.99	0.43
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.83	0.43
2:C:132:LEU:HD22	2:C:155:LEU:HD23	1.99	0.43
2:C:138:LEU:HA	2:C:139:PRO:HD3	1.89	0.43
1:A:328:LEU:HD12	1:A:331:ILE:HG21	2.01	0.43
1:A:365:ASP:OD2	1:A:367:ARG:HD3	2.19	0.43
1:A:400:MET:HA	1:A:403:TYR:CD2	2.54	0.43
1:A:451:VAL:O	1:A:455:MET:HG2	2.18	0.43
2:C:144:PRO:O	2:C:148:VAL:HG23	2.18	0.43
1:A:522:VAL:HG22	1:A:526:ILE:HG23	2.00	0.43
1:A:523:VAL:HG23	2:C:521:HIS:HB3	2.01	0.43
2:C:228:CYS:SG	2:C:399:ARG:HG2	2.58	0.43
2:C:290:THR:HG23	2:C:291:THR:N	2.34	0.43
1:A:317:PHE:N	1:A:318:PRO:CD	2.80	0.43
1:A:231:THR:HG23	1:A:423:ARG:HH12	1.84	0.43
2:C:251:LEU:HG	2:C:256:ILE:O	2.19	0.43
1:A:365:ASP:OD2	1:A:365:ASP:N	2.52	0.43
2:C:365:ASP:OD2	2:C:367:ARG:HD3	2.19	0.43
1:A:207:LYS:O	1:A:211:GLU:HG3	2.19	0.43
1:A:251:LEU:HG	1:A:256:ILE:O	2.19	0.42
1:A:290:THR:HG23	1:A:291:THR:N	2.34	0.42
1:A:309:LEU:HD12	1:A:338:PRO:HB2	2.01	0.42
2:C:231:THR:HG23	2:C:423:ARG:HH12	1.84	0.42
2:C:365:ASP:OD2	2:C:365:ASP:N	2.52	0.42
1:A:345:LEU:HD21	1:A:478:VAL:HG21	2.01	0.42
1:A:479:ILE:O	1:A:512:HIS:HB2	2.20	0.42
2:C:355:LYS:HD2	2:C:355:LYS:N	2.34	0.42
2:C:465:ILE:N	2:C:466:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:LYS:O	2:C:211:GLU:HG3	2.18	0.42
2:C:309:LEU:HD12	2:C:338:PRO:HB2	2.01	0.42
1:A:261:ILE:HD12	1:A:309:LEU:O	2.19	0.42
2:C:261:ILE:HD12	2:C:309:LEU:O	2.20	0.42
2:C:283:ARG:HB3	2:C:283:ARG:CZ	2.50	0.42
1:A:355:LYS:N	1:A:355:LYS:HD2	2.34	0.42
1:A:283:ARG:HB3	1:A:283:ARG:CZ	2.50	0.41
1:A:296:LEU:HD12	1:A:296:LEU:N	2.34	0.41
1:A:486:LEU:HD22	1:A:486:LEU:N	2.36	0.41
2:C:317:PHE:HB3	2:C:318:PRO:HD3	2.02	0.41
2:C:440:GLU:O	2:C:444:ILE:HG13	2.19	0.41
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.89	0.41
1:A:523:VAL:HB	2:C:521:HIS:ND1	2.36	0.41
1:A:525:GLU:H	1:A:525:GLU:HG3	1.67	0.41
1:A:244:LEU:HD13	1:A:278:PHE:CE1	2.56	0.41
2:C:345:LEU:HD21	2:C:478:VAL:HG21	2.02	0.41
2:C:319:HIS:ND1	2:C:471:MET:HG2	2.35	0.41
2:C:525:GLU:H	2:C:525:GLU:HG3	1.68	0.41
1:A:191:TYR:CD1	1:A:429:VAL:HG11	2.56	0.41
1:A:230:THR:HG21	1:A:402:GLN:HE22	1.86	0.41
1:A:425:GLY:O	1:A:429:VAL:HG23	2.21	0.41
2:C:399:ARG:H	2:C:399:ARG:HG3	1.55	0.41
1:A:423:ARG:HA	1:A:424:PRO:HD3	1.84	0.41
1:A:288:ASP:OD2	1:A:290:THR:HG22	2.21	0.41
1:A:317:PHE:HB3	1:A:318:PRO:HD3	2.02	0.41
1:A:335:TYR:C	1:A:336:LYS:HG3	2.46	0.41
1:A:497:LYS:HB3	1:A:497:LYS:HE3	1.87	0.41
2:C:244:LEU:HD13	2:C:278:PHE:CE1	2.55	0.41
2:C:367:ARG:O	2:C:369:PRO:HD3	2.21	0.41
2:C:486:LEU:HD22	2:C:486:LEU:N	2.35	0.41
1:A:440:GLU:O	1:A:444:ILE:HG13	2.20	0.41
1:A:319:HIS:ND1	1:A:471:MET:HG2	2.36	0.40
1:A:393:TYR:CD1	1:A:398:LEU:HB3	2.56	0.40
2:C:479:ILE:O	2:C:512:HIS:HB2	2.20	0.40
2:C:484:LYS:H	2:C:484:LYS:HG2	1.67	0.40
2:C:537:LEU:HD12	2:C:538:LYS:N	2.37	0.40
2:C:335:TYR:C	2:C:336:LYS:HG3	2.46	0.40
2:C:425:GLY:O	2:C:429:VAL:HG23	2.21	0.40
2:C:446:SER:O	2:C:450:ILE:HG12	2.21	0.40
2:C:230:THR:HG21	2:C:402:GLN:HE22	1.85	0.40
1:A:191:TYR:O	1:A:426:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HA	1:A:338:PRO:HD3	1.93	0.40
2:C:191:TYR:CD1	2:C:429:VAL:HG11	2.56	0.40
1:A:185:THR:O	1:A:188:TYR:HB3	2.22	0.40
2:C:191:TYR:O	2:C:426:ALA:HB2	2.20	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	421/497 (85%)	381 (90%)	35 (8%)	5 (1%)	10	37
2	C	420/497 (84%)	379 (90%)	36 (9%)	5 (1%)	10	37
All	All	841/994 (85%)	760 (90%)	71 (8%)	10 (1%)	10	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ALA
2	C	158	LEU
2	C	267	ALA
1	A	158	LEU
1	A	172	ALA
1	A	347	SER
2	C	172	ALA
2	C	347	SER
1	A	233	SER
2	C	233	SER

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	360/420 (86%)	343 (95%)	17 (5%)	23	52
2	C	361/421 (86%)	344 (95%)	17 (5%)	23	52
All	All	721/841 (86%)	687 (95%)	34 (5%)	23	52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ILE
1	A	180	LEU
1	A	183	LEU
1	A	186	ILE
1	A	230	THR
1	A	251	LEU
1	A	336	LYS
1	A	355	LYS
1	A	367	ARG
1	A	399	ARG
1	A	438	MET
1	A	445	GLU
1	A	471	MET
1	A	488	ILE
1	A	512	HIS
1	A	523	VAL
1	A	525	GLU
2	C	149	ILE
2	C	180	LEU
2	C	183	LEU
2	C	186	ILE
2	C	230	THR
2	C	251	LEU
2	C	336	LYS
2	C	355	LYS
2	C	367	ARG
2	C	399	ARG

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Mol	Chain	Res	Type
2	C	438	MET
2	C	445	GLU
2	C	471	MET
2	C	488	ILE
2	C	512	HIS
2	C	523	VAL
2	C	525	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	198	HIS
1	A	284	HIS
1	A	333	GLN
1	A	406	ASN
1	A	487	ASN
1	A	501	HIS
2	C	184	GLN
2	C	284	HIS
2	C	333	GLN
2	C	406	ASN
2	C	487	ASN
2	C	501	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
1	LLP	A	380	1	23,24,25	1.73	3 (13%)	25,32,34	1.79	4 (16%)

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
1	LLP	A	380	1	-	6/16/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	LLP	O3-C3	-5.89	1.23	1.36
1	A	380	LLP	C2-N1	2.50	1.38	1.33
1	A	380	LLP	C4'-NZ	2.01	1.33	1.27

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	LLP	OP4-C5'-C5	6.35	121.27	109.36
1	A	380	LLP	C4-C4'-NZ	-3.06	109.91	124.04
1	A	380	LLP	CE-NZ-C4'	-2.77	109.85	118.72
1	A	380	LLP	C5-C6-N1	-2.22	120.23	123.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	380	LLP	C4-C4'-NZ-CE
1	A	380	LLP	O-C-CA-CB
1	A	380	LLP	C6-C5-C5'-OP4
1	A	380	LLP	C4-C5-C5'-OP4
1	A	380	LLP	CD-CE-NZ-C4'
1	A	380	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	380	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	PO4	C	2	-	4,4,4	0.97	0	6,6,6	0.46	0
3	PO4	A	1	-	4,4,4	0.97	0	6,6,6	0.48	0
3	PO4	C	1[B]	-	4,4,4	0.93	0	6,6,6	0.50	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	425/497 (85%)	0.15	6 (1%)	73 53	61, 108, 197, 303	0
2	C	424/497 (85%)	-0.08	1 (0%)	91 84	68, 127, 214, 288	0
All	All	849/994 (85%)	0.04	7 (0%)	82 66	61, 118, 210, 303	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	3.4
1	A	310	LEU	3.2
1	A	414	TYR	3.0
1	A	312	GLY	2.9
1	A	331	ILE	2.4
1	A	322	ALA	2.4
2	C	521	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	380	24/25	0.97	0.06	25,84,112,143	0

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	PO4	C	2	5/5	0.91	0.13	70,107,121,169	0
3	PO4	A	1	5/5	0.92	0.11	62,80,88,90	0
3	PO4	C	1[B]	5/5	0.93	0.12	69,89,143,163	0

6.5 Other polymers [i](#)

There are no such residues in this entry.