Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 05:41 AM EDT

PDB ID	:	3MAF
Title	:	Crystal structure of StSPL (asymmetric form)
Authors	:	Bourquin, F.; Grutter, M.G.; Capitani, G.
Deposited on	:	2010-03-23
Resolution	:	2.97 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 (i) 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 (1)) were used in the production of this report:

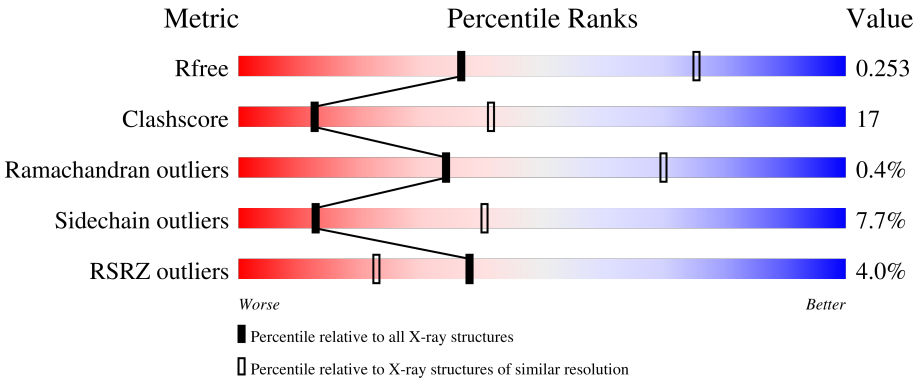
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	518	5% 56% 26% · 15%
2	B	518	2% 52% 21% · 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6479 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
1	A	441	Total	C	N	O	P	S	0	0	0
			3362	2152	586	611	1	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q67PY4
A	-3	GLY	-	expression tag	UNP Q67PY4
A	-2	GLY	-	expression tag	UNP Q67PY4
A	-1	SER	-	expression tag	UNP Q67PY4
A	0	ARG	-	expression tag	UNP Q67PY4
A	1	SER	-	expression tag	UNP Q67PY4
A	508	HIS	-	expression tag	UNP Q67PY4
A	509	HIS	-	expression tag	UNP Q67PY4
A	510	HIS	-	expression tag	UNP Q67PY4
A	511	HIS	-	expression tag	UNP Q67PY4
A	512	HIS	-	expression tag	UNP Q67PY4
A	513	HIS	-	expression tag	UNP Q67PY4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			2985	1911	523	540	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	expression tag	UNP Q67PY4
B	-3	GLY	-	expression tag	UNP Q67PY4
B	-2	GLY	-	expression tag	UNP Q67PY4
B	-1	SER	-	expression tag	UNP Q67PY4

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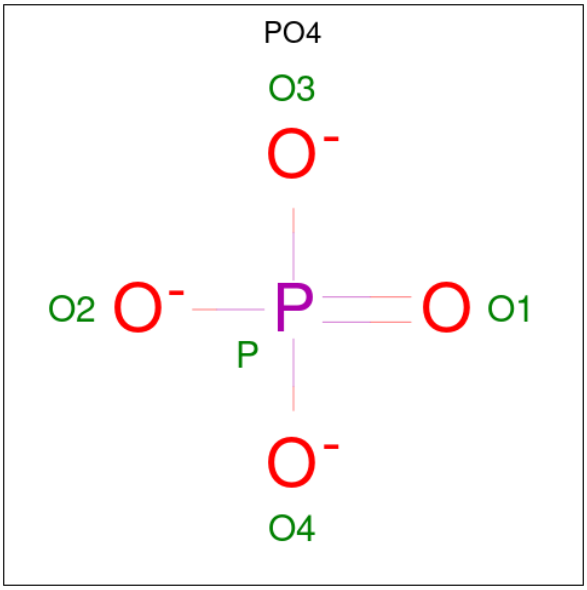
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP Q67PY4
B	1	SER	-	expression tag	UNP Q67PY4
B	508	HIS	-	expression tag	UNP Q67PY4
B	509	HIS	-	expression tag	UNP Q67PY4
B	510	HIS	-	expression tag	UNP Q67PY4
B	511	HIS	-	expression tag	UNP Q67PY4
B	512	HIS	-	expression tag	UNP Q67PY4
B	513	HIS	-	expression tag	UNP Q67PY4

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	65	Total O 65 65	0	0

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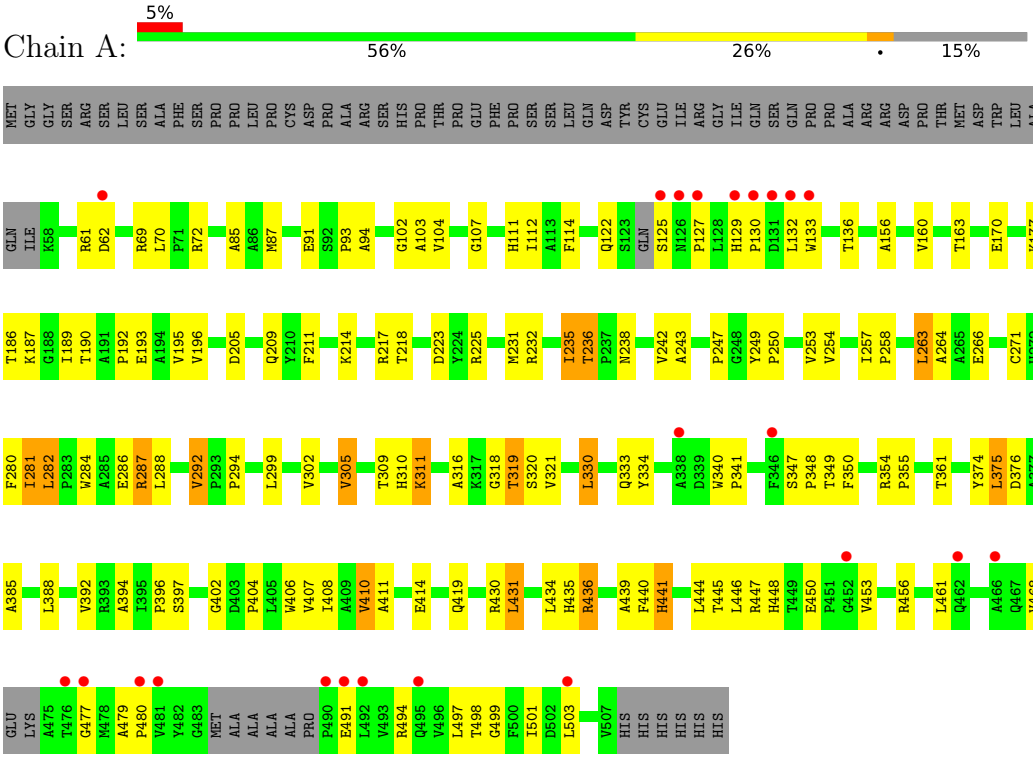
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	61	Total	O	0	0
			61	61		

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.

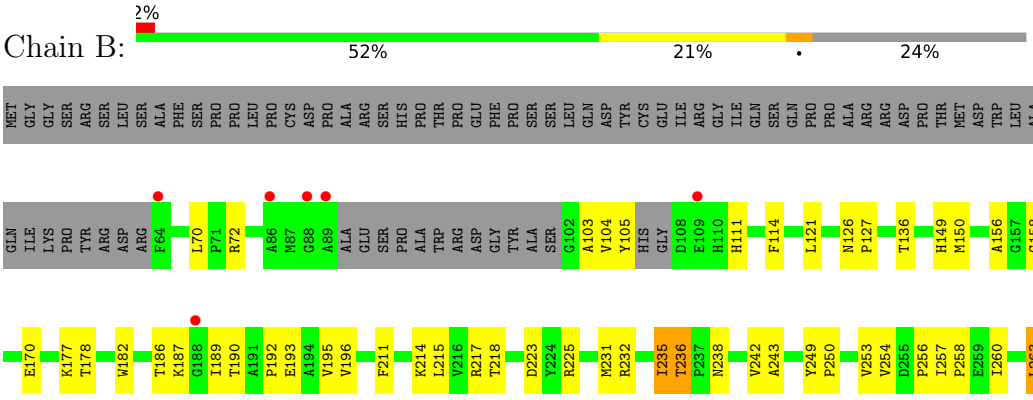
• Molecule 1: sphingosine-1-phosphate lyase

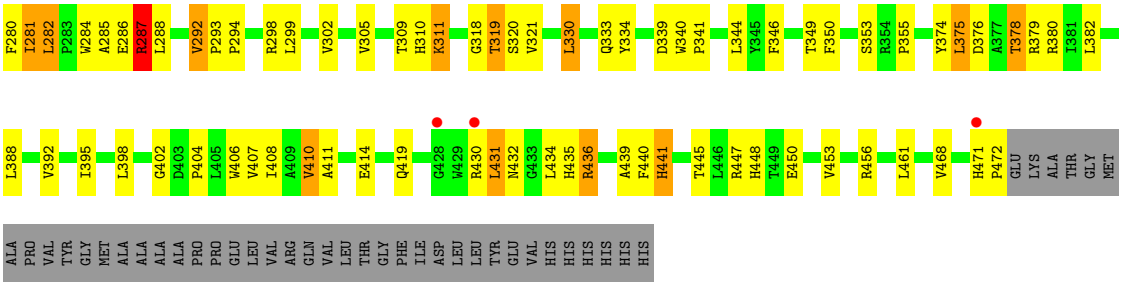
Chain A:



• Molecule 2: sphingosine-1-phosphate lyase

Chain B:




F280 I281 L282 P283 W284 A285 E286 R287 L288 V292 P293 P294 R298 L299 V302 V305 T309 H310 K311 G318 T319 S320 V321 L330 Q333 Y334 D339 W340 P341 L344 Y345 F346 T349 F350 S353 R354 P355 Y374 L375 D376 A377 T378 R379 R380 I381 L382
L388 V392 I395 L398 G402 D403 P404 L405 W406 V407 I408 A409 V410 A411 E414 Q419 G428 W429 R430 L431 N432 G433 L434 H435 R436 A439 F440 H441 T445 L446 R447 H448 T449 E450 V453 R456 L461 V468 H471 P472 GLU LYS ALA THR GLY MET
ALA PRO VAL TYR GLY MET ALA ALA ALA ALA PRO PRO GLU LEU VAL ARG GLN VAL LEU THR GLY PHE ILE ASP LEU LEU TYR GLU VAL HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.19Å 84.90Å 131.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.66 – 2.97 29.89 – 2.97	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.66-2.97) 98.9 (29.89-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	8.27 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.4_29	Depositor
R, R_{free}	0.200 , 0.265 0.196 , 0.253	Depositor DCC
R_{free} test set	989 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6479	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, LLP, CL

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	0.34	0/3430	0.65	9/4681 (0.2%)
2	B	0.34	0/3067	0.67	9/4188 (0.2%)
All	All	0.34	0/6497	0.66	18/8869 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	ARG	NE-CZ-NH1	-12.54	114.03	120.30
2	B	379	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	456	ARG	NE-CZ-NH1	-11.53	114.54	120.30
1	A	379	ARG	NE-CZ-NH2	11.47	126.03	120.30
2	B	456	ARG	NE-CZ-NH2	-11.45	114.57	120.30
2	B	287	ARG	NE-CZ-NH1	-11.43	114.58	120.30
2	B	379	ARG	NE-CZ-NH1	11.29	125.94	120.30
2	B	287	ARG	NE-CZ-NH2	11.13	125.86	120.30
2	B	456	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	287	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	A	287	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	456	ARG	NE-CZ-NH2	10.11	125.36	120.30
1	A	379	ARG	CD-NE-CZ	5.97	131.96	123.60
2	B	456	ARG	CD-NE-CZ	5.81	131.73	123.60
1	A	287	ARG	CD-NE-CZ	5.63	131.48	123.60
2	B	379	ARG	CD-NE-CZ	5.62	131.47	123.60
2	B	287	ARG	CD-NE-CZ	5.51	131.32	123.60
1	A	456	ARG	CD-NE-CZ	5.41	131.17	123.60

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	3362	0	3291	122	0
2	B	2985	0	2938	105	0
3	A	1	0	0	0	0
4	B	5	0	0	0	0
5	A	65	0	0	3	0
5	B	61	0	0	3	0
All	All	6479	0	6229	211	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 17.

All (211) 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:436:ARG:HG3	2:B:436:ARG:HH11	1.23	1.03
1:A:236:THR:HG23	1:A:238:ASN:H	1.25	1.01
2:B:236:THR:HG23	2:B:238:ASN:H	1.24	1.01
1:A:436:ARG:HH11	1:A:436:ARG:HG3	1.23	1.00
2:B:127:PRO:HG3	2:B:136:THR:HG21	1.48	0.95
2:B:445:THR:HG22	2:B:447:ARG:H	1.37	0.90
1:A:445:THR:HG22	1:A:447:ARG:H	1.39	0.86
2:B:434:LEU:HD11	2:B:441:HIS:HB3	1.58	0.86
1:A:434:LEU:HD11	1:A:441:HIS:HB3	1.57	0.84
1:A:374:TYR:O	1:A:378:THR:HG22	1.82	0.79
1:A:411:ALA:HB2	1:A:439:ALA:HB2	1.65	0.78
2:B:411:ALA:HB2	2:B:439:ALA:HB2	1.66	0.77
2:B:436:ARG:HH11	2:B:436:ARG:CG	1.99	0.75
2:B:374:TYR:O	2:B:378:THR:HG22	1.86	0.75
1:A:436:ARG:HH11	1:A:436:ARG:CG	2.00	0.75
2:B:284:TRP:HB3	2:B:375:LEU:HD13	1.69	0.73
1:A:284:TRP:HB3	1:A:375:LEU:HD13	1.69	0.73
2:B:284:TRP:O	2:B:288:LEU:HB2	1.89	0.73
2:B:158:GLY:HA2	5:B:678:HOH:O	1.88	0.72
2:B:309:THR:OG1	2:B:319:THR:HG23	1.89	0.72
2:B:431:LEU:H	2:B:431:LEU:HD23	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD23	1:A:431:LEU:H	1.54	0.71
1:A:309:THR:OG1	1:A:319:THR:HG23	1.91	0.70
1:A:394:ALA:O	1:A:396:PRO:HD3	1.92	0.69
2:B:310:HIS:CE1	2:B:311:LYS:HG3	2.28	0.69
2:B:196:VAL:HG12	2:B:243:ALA:HB3	1.73	0.69
2:B:284:TRP:HB2	2:B:378:THR:HG21	1.75	0.69
1:A:284:TRP:O	1:A:288:LEU:HB2	1.94	0.68
1:A:284:TRP:HB2	1:A:378:THR:HG21	1.75	0.68
1:A:350:PHE:HE2	2:B:350:PHE:HE2	1.42	0.67
2:B:436:ARG:HG3	2:B:436:ARG:NH1	2.03	0.67
1:A:196:VAL:HG12	1:A:243:ALA:HB3	1.77	0.66
2:B:126:ASN:HD21	2:B:353:SER:HB2	1.62	0.65
1:A:281:ILE:HD11	1:A:406:TRP:CZ3	2.33	0.64
2:B:225:ARG:HD2	2:B:254:VAL:O	1.96	0.64
1:A:225:ARG:HD2	1:A:254:VAL:O	1.96	0.64
1:A:69:ARG:HD3	2:B:149:HIS:CE1	2.35	0.62
1:A:127:PRO:HD3	1:A:354:ARG:O	1.99	0.62
2:B:281:ILE:HD11	2:B:406:TRP:CZ3	2.35	0.62
2:B:450:GLU:HB2	2:B:453:VAL:HG21	1.83	0.61
1:A:419:GLN:HG3	1:A:468:VAL:HG22	1.82	0.61
1:A:374:TYR:O	1:A:378:THR:CG2	2.48	0.60
2:B:419:GLN:HG3	2:B:468:VAL:HG22	1.82	0.60
1:A:350:PHE:CE2	2:B:350:PHE:HE2	2.20	0.59
2:B:374:TYR:O	2:B:378:THR:CG2	2.51	0.58
1:A:319:THR:HG21	5:A:697:HOH:O	2.02	0.58
2:B:196:VAL:O	2:B:217:ARG:HA	2.04	0.58
1:A:236:THR:CG2	1:A:238:ASN:H	2.08	0.58
1:A:450:GLU:HB2	1:A:453:VAL:HG21	1.85	0.58
2:B:471:HIS:N	2:B:472:PRO:HD3	2.19	0.57
1:A:350:PHE:CE2	2:B:350:PHE:CE2	2.93	0.57
1:A:211:PHE:HZ	1:A:350:PHE:HZ	1.53	0.57
2:B:431:LEU:H	2:B:431:LEU:CD2	2.16	0.57
1:A:471:HIS:N	1:A:472:PRO:HD3	2.19	0.56
1:A:196:VAL:O	1:A:217:ARG:HA	2.06	0.56
1:A:294:PRO:HB2	1:A:299:LEU:HD21	1.87	0.56
1:A:497:LEU:O	1:A:501:ILE:HG13	2.06	0.56
2:B:310:HIS:ND1	2:B:311:LYS:N	2.54	0.56
2:B:193:GLU:HG2	2:B:214:LYS:HB3	1.87	0.55
2:B:211:PHE:HZ	2:B:350:PHE:HZ	1.53	0.55
2:B:105:TYR:CD1	2:B:311:LYS:HA	2.41	0.55
1:A:193:GLU:HG2	1:A:214:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:H	1:A:431:LEU:CD2	2.19	0.55
1:A:122:GLN:HA	1:A:122:GLN:HE21	1.72	0.54
2:B:294:PRO:HB2	2:B:299:LEU:HD21	1.89	0.54
2:B:190:THR:C	2:B:192:PRO:HD3	2.29	0.54
1:A:379:ARG:HD2	5:A:636:HOH:O	2.07	0.53
1:A:497:LEU:HD21	2:B:344:LEU:HB3	1.90	0.53
1:A:190:THR:C	1:A:192:PRO:HD3	2.29	0.53
1:A:350:PHE:HE2	2:B:350:PHE:CE2	2.25	0.53
1:A:127:PRO:HD2	1:A:354:ARG:HG3	1.91	0.52
1:A:235:ILE:HD12	1:A:236:THR:N	2.24	0.52
1:A:430:ARG:HD2	1:A:430:ARG:N	2.24	0.52
1:A:477:GLY:O	1:A:480:PRO:HD2	2.09	0.52
2:B:236:THR:CG2	2:B:238:ASN:H	2.10	0.52
2:B:235:ILE:HD12	2:B:236:THR:N	2.25	0.52
1:A:499:GLY:O	1:A:503:LEU:HG	2.10	0.51
1:A:195:VAL:HB	1:A:242:VAL:HG12	1.93	0.51
1:A:341:PRO:HA	2:B:435:HIS:O	2.11	0.51
1:A:122:GLN:O	1:A:125:SER:HB3	2.10	0.51
2:B:195:VAL:HB	2:B:242:VAL:HG12	1.93	0.51
1:A:501:ILE:HD11	2:B:346:PHE:HB2	1.93	0.50
2:B:70:LEU:HB2	5:B:612:HOH:O	2.11	0.50
1:A:436:ARG:HG3	1:A:436:ARG:NH1	2.04	0.50
2:B:436:ARG:CG	2:B:436:ARG:NH1	2.64	0.50
2:B:105:TYR:CE1	2:B:311:LYS:HG2	2.47	0.50
2:B:187:LYS:HB2	2:B:189:ILE:HG13	1.93	0.50
1:A:436:ARG:CG	1:A:436:ARG:NH1	2.65	0.50
1:A:435:HIS:O	2:B:341:PRO:HA	2.12	0.49
2:B:376:ASP:O	2:B:380:ARG:HG3	2.13	0.49
2:B:448:HIS:HA	2:B:453:VAL:HG11	1.94	0.49
2:B:218:THR:HG21	2:B:231:MET:HA	1.95	0.49
1:A:170:GLU:OE2	1:A:349:THR:HB	2.14	0.48
1:A:178:THR:OG1	1:A:333:GLN:HB2	2.12	0.48
2:B:388:LEU:O	2:B:392:VAL:HG23	2.13	0.48
1:A:70:LEU:HD22	2:B:150:MET:HE2	1.96	0.48
1:A:192:PRO:HG3	5:A:719:HOH:O	2.14	0.48
2:B:156:ALA:HB3	2:B:160:VAL:HG23	1.95	0.48
2:B:430:ARG:N	2:B:430:ARG:HD2	2.28	0.48
1:A:340:TRP:CD1	1:A:341:PRO:HD2	2.48	0.48
1:A:127:PRO:O	1:A:130:PRO:HD3	2.14	0.47
1:A:376:ASP:O	1:A:380:ARG:HG3	2.14	0.47
2:B:249:TYR:N	2:B:250:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:CD	1:A:354:ARG:HG3	2.44	0.47
1:A:264:ALA:CB	1:A:271:CYS:HB2	2.45	0.47
1:A:479:ALA:HB3	1:A:480:PRO:HD3	1.95	0.47
2:B:156:ALA:CB	2:B:160:VAL:HG23	2.45	0.47
2:B:340:TRP:CD1	2:B:341:PRO:HD2	2.49	0.47
2:B:170:GLU:OE2	2:B:349:THR:HB	2.15	0.47
2:B:286:GLU:C	2:B:288:LEU:H	2.19	0.47
1:A:187:LYS:HB2	1:A:189:ILE:HG13	1.97	0.46
2:B:288:LEU:HD12	2:B:288:LEU:HA	1.79	0.46
1:A:93:PRO:O	1:A:94:ALA:C	2.54	0.46
1:A:218:THR:HG21	1:A:231:MET:HA	1.97	0.46
1:A:280:PHE:CZ	1:A:309:THR:HG22	2.51	0.46
1:A:232:ARG:HA	1:A:263:LEU:HD11	1.98	0.46
2:B:264:ALA:CB	2:B:271:CYS:HB2	2.45	0.46
1:A:281:ILE:C	1:A:281:ILE:HD12	2.35	0.46
1:A:330:LEU:HD13	1:A:334:TYR:OH	2.16	0.46
1:A:127:PRO:HG3	1:A:136:THR:HG21	1.97	0.45
1:A:431:LEU:CD2	1:A:431:LEU:N	2.80	0.45
1:A:182:TRP:O	1:A:186:THR:HB	2.17	0.45
1:A:273:VAL:HB	1:A:305:VAL:HB	1.97	0.45
1:A:156:ALA:CB	1:A:160:VAL:HG23	2.47	0.45
2:B:330:LEU:HD13	2:B:334:TYR:OH	2.17	0.45
1:A:163:THR:HG21	1:A:349:THR:HG22	1.98	0.45
1:A:355:PRO:HG3	2:B:318:GLY:HA3	1.99	0.45
1:A:111:HIS:O	1:A:114:PHE:HB3	2.17	0.45
2:B:410:VAL:HG13	2:B:440:PHE:CE1	2.52	0.45
2:B:450:GLU:HB2	2:B:453:VAL:CG2	2.45	0.45
2:B:232:ARG:HA	2:B:263:LEU:HD11	1.99	0.45
2:B:431:LEU:CD2	2:B:431:LEU:N	2.79	0.45
1:A:104:VAL:O	1:A:445:THR:HG21	2.16	0.45
1:A:249:TYR:N	1:A:250:PRO:CD	2.79	0.45
1:A:299:LEU:HB2	1:A:302:VAL:HG23	1.99	0.45
1:A:310:HIS:HB3	1:A:319:THR:HG22	1.99	0.45
1:A:388:LEU:C	1:A:388:LEU:HD23	2.37	0.45
1:A:388:LEU:O	1:A:392:VAL:HG23	2.17	0.45
2:B:150:MET:O	2:B:150:MET:HG2	2.16	0.44
2:B:281:ILE:C	2:B:281:ILE:HD12	2.37	0.44
1:A:448:HIS:HA	1:A:453:VAL:HG11	1.99	0.44
2:B:282:LEU:HD12	2:B:282:LEU:HA	1.80	0.44
2:B:163:THR:HG21	2:B:349:THR:HG22	1.99	0.44
2:B:287:ARG:NH1	5:B:680:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:HD2	1:A:319:THR:O	1.99	0.44
1:A:87:MET:O	1:A:91:GLU:HG3	2.17	0.44
1:A:156:ALA:HB3	1:A:160:VAL:HG23	2.00	0.44
1:A:311:LLP:O3	1:A:311:LLP:NZ	2.50	0.44
2:B:258:PRO:HA	2:B:299:LEU:HD13	2.00	0.44
1:A:186:THR:HG22	1:A:187:LYS:HG2	1.99	0.44
1:A:479:ALA:N	1:A:480:PRO:CD	2.81	0.44
1:A:396:PRO:HA	1:A:397:SER:HA	1.30	0.43
1:A:431:LEU:HD12	1:A:440:PHE:CD1	2.53	0.43
1:A:282:LEU:HG	1:A:292:VAL:HG21	1.99	0.43
2:B:178:THR:OG1	2:B:333:GLN:HB2	2.18	0.43
1:A:410:VAL:HG13	1:A:440:PHE:CE1	2.53	0.43
1:A:450:GLU:HB2	1:A:453:VAL:CG2	2.49	0.43
2:B:104:VAL:O	2:B:445:THR:HG21	2.18	0.43
2:B:292:VAL:HA	2:B:293:PRO:HD3	1.79	0.43
2:B:402:GLY:C	2:B:404:PRO:HD3	2.38	0.43
2:B:310:HIS:HD2	2:B:319:THR:H	1.66	0.43
1:A:107:GLY:HA2	1:A:112:ILE:HD11	2.00	0.43
1:A:258:PRO:HA	1:A:299:LEU:HD13	2.01	0.43
1:A:445:THR:CG2	1:A:446:LEU:N	2.82	0.43
1:A:129:HIS:HB3	1:A:132:LEU:HD12	2.01	0.43
1:A:402:GLY:C	1:A:404:PRO:HD3	2.39	0.42
2:B:196:VAL:HG22	2:B:215:LEU:HD11	2.00	0.42
1:A:498:THR:HG23	2:B:334:TYR:CD2	2.54	0.42
2:B:431:LEU:HD12	2:B:440:PHE:CD1	2.54	0.42
1:A:288:LEU:HD12	1:A:288:LEU:HA	1.79	0.42
2:B:111:HIS:O	2:B:114:PHE:HB3	2.20	0.42
2:B:320:SER:OG	2:B:321:VAL:N	2.53	0.42
1:A:286:GLU:C	1:A:288:LEU:H	2.21	0.42
2:B:186:THR:HG22	2:B:187:LYS:HG2	2.01	0.42
2:B:282:LEU:HG	2:B:292:VAL:HG21	2.00	0.42
2:B:395:ILE:HD12	2:B:398:LEU:HD12	2.00	0.42
2:B:404:PRO:HB3	2:B:407:VAL:O	2.19	0.42
1:A:247:PRO:HD3	1:A:278:GLY:HA3	2.02	0.42
2:B:182:TRP:O	2:B:186:THR:HB	2.20	0.42
2:B:286:GLU:OE1	2:B:298:ARG:NH1	2.53	0.42
1:A:347:SER:HA	1:A:348:PRO:HD3	1.86	0.42
1:A:436:ARG:HD2	2:B:339:ASP:HB2	2.01	0.42
2:B:404:PRO:HB2	2:B:408:ILE:HD13	2.02	0.42
1:A:318:GLY:HA3	2:B:355:PRO:HG3	2.02	0.42
1:A:122:GLN:HA	1:A:122:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:LEU:HD13	2:B:375:LEU:HA	1.83	0.41
1:A:434:LEU:HB3	2:B:341:PRO:O	2.20	0.41
1:A:85:ALA:HB2	2:B:121:LEU:HD13	2.01	0.41
1:A:205:ASP:O	1:A:209:GLN:HG3	2.20	0.41
2:B:284:TRP:CE3	2:B:375:LEU:HD22	2.56	0.41
1:A:182:TRP:CH2	1:A:187:LYS:HE2	2.56	0.41
1:A:125:SER:HA	1:A:133:TRP:CE2	2.55	0.41
1:A:266:GLU:O	1:A:266:GLU:HG2	2.20	0.41
2:B:182:TRP:CH2	2:B:187:LYS:HE2	2.56	0.41
2:B:285:ALA:HB2	2:B:382:LEU:HD11	2.01	0.41
2:B:280:PHE:CZ	2:B:309:THR:HG22	2.56	0.41
2:B:299:LEU:HB2	2:B:302:VAL:HG23	2.03	0.41
1:A:257:ILE:N	1:A:258:PRO:CD	2.83	0.41
1:A:320:SER:OG	1:A:321:VAL:N	2.54	0.41
1:A:385:ALA:HB2	1:A:444:LEU:HD12	2.02	0.41
1:A:404:PRO:HB3	1:A:407:VAL:O	2.21	0.41
2:B:310:HIS:ND1	2:B:311:LYS:HG3	2.36	0.41
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.83	0.40
1:A:129:HIS:CB	1:A:132:LEU:HD12	2.51	0.40
2:B:257:ILE:N	2:B:258:PRO:CD	2.84	0.40
1:A:102:GLY:O	1:A:104:VAL:N	2.54	0.40
1:A:282:LEU:HD12	1:A:282:LEU:HA	1.82	0.40
1:A:404:PRO:HB2	1:A:408:ILE:HD13	2.04	0.40
2:B:432:ASN:HB2	2:B:441:HIS:ND1	2.37	0.40
1:A:316:ALA:HB3	1:A:361:THR:OG1	2.22	0.40
2:B:256:PRO:O	2:B:260:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	432/518 (83%)	407 (94%)	24 (6%)	1 (0%)	47 80
2	B	389/518 (75%)	363 (93%)	24 (6%)	2 (0%)	29 66
All	All	821/1036 (79%)	770 (94%)	48 (6%)	3 (0%)	34 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	311	LYS
2	B	103	ALA
1	A	103	ALA

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	331/397 (83%)	305 (92%)	26 (8%)	12 39
2	B	296/398 (74%)	274 (93%)	22 (7%)	13 42
All	All	627/795 (79%)	579 (92%)	48 (8%)	13 40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	62	ASP
1	A	72	ARG
1	A	177	LYS
1	A	223	ASP
1	A	235	ILE
1	A	236	THR
1	A	253	VAL
1	A	263	LEU
1	A	281	ILE
1	A	282	LEU
1	A	287	ARG
1	A	292	VAL

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Mol	Chain	Res	Type
1	A	305	VAL
1	A	319	THR
1	A	330	LEU
1	A	375	LEU
1	A	378	THR
1	A	410	VAL
1	A	414	GLU
1	A	431	LEU
1	A	436	ARG
1	A	441	HIS
1	A	461	LEU
1	A	491	GLU
1	A	494	ARG
2	B	72	ARG
2	B	177	LYS
2	B	223	ASP
2	B	235	ILE
2	B	236	THR
2	B	253	VAL
2	B	263	LEU
2	B	281	ILE
2	B	282	LEU
2	B	287	ARG
2	B	292	VAL
2	B	305	VAL
2	B	319	THR
2	B	330	LEU
2	B	375	LEU
2	B	378	THR
2	B	410	VAL
2	B	414	GLU
2	B	431	LEU
2	B	436	ARG
2	B	441	HIS
2	B	461	LEU

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

Mol	Chain	Res	Type
1	A	122	GLN
1	A	310	HIS
2	B	67	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	311	1	23,24,25	1.69	4 (17%)	25,32,34	1.70	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	311	1	-	5/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	LLP	O3-C3	-5.59	1.24	1.37
1	A	311	LLP	C4-C4'	2.48	1.51	1.46
1	A	311	LLP	C2-N1	2.27	1.38	1.33
1	A	311	LLP	C4'-NZ	2.07	1.34	1.27

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	LLP	OP4-C5'-C5	6.07	120.93	109.35
1	A	311	LLP	C4-C4'-NZ	-3.25	109.37	124.31
1	A	311	LLP	OP3-P-OP2	2.07	115.56	107.64
1	A	311	LLP	C5-C6-N1	-2.07	120.36	123.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	311	LLP	O-C-CA-CB
1	A	311	LLP	C4-C4'-NZ-CE
1	A	311	LLP	C6-C5-C5'-OP4
1	A	311	LLP	C4-C5-C5'-OP4
1	A	311	LLP	CD-CE-NZ-C4'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	311	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	B	514	-	4,4,4	0.74	0	6,6,6	0.63	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

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, 95^{th} 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	440/518 (84%)	-0.01	24 (5%) 25 14	15, 29, 64, 85	0
2	B	395/518 (76%)	-0.15	9 (2%) 60 40	15, 28, 51, 71	0
All	All	835/1036 (80%)	-0.07	33 (3%) 38 23	15, 29, 59, 85	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	89	ALA	5.1
1	A	126	ASN	4.2
2	B	88	GLY	3.8
2	B	64	PHE	3.4
1	A	491	GLU	3.4
1	A	132	LEU	3.3
1	A	130	PRO	3.2
1	A	346	PHE	3.2
1	A	466	ALA	2.9
1	A	133	TRP	2.9
1	A	131	ASP	2.9
2	B	188	GLY	2.9
1	A	480	PRO	2.7
1	A	127	PRO	2.7
1	A	481	VAL	2.7
1	A	490	PRO	2.7
2	B	471	HIS	2.7
1	A	62	ASP	2.5
1	A	338	ALA	2.5
1	A	492	LEU	2.5
2	B	430	ARG	2.4
1	A	125	SER	2.4
2	B	109	GLU	2.3
1	A	503	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	495	GLN	2.3
1	A	452	GLY	2.3
1	A	129	HIS	2.2
1	A	462	GLN	2.2
2	B	428	GLY	2.1
2	B	86	ALA	2.1
1	A	469	ARG	2.1
1	A	477	GLY	2.1
1	A	476	THR	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, 95^{th} 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	311	24/25	0.97	0.16	17,29,34,43	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	CL	A	514	1/1	0.81	0.30	62,62,62,62	0
4	PO4	B	514	5/5	0.83	0.24	31,37,83,90	0

6.5 Other polymers (i)

There are no such residues in this entry.