



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:04 PM EDT

PDB ID : 7KFK
Title : Crystal structure of LILRB1 D3D4 domain in complex with Plasmodium RIFIN (PF3D7_1373400) V2 domain
Authors : Xu, K.; Kwong, P.D.
Deposited on : 2020-10-14
Resolution : 2.63 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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

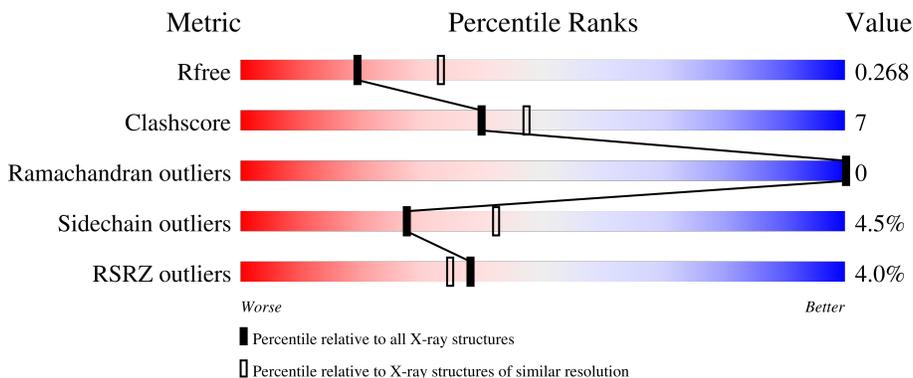
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	233	 2% 74% 13% • 11%
1	B	233	 4% 70% 18% • 11%
2	C	151	 2% 68% 18% • 13%
2	E	151	 7% 68% 13% •• 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5150 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 Isoform 2 of Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1570	990	266	308	6	0	0	0
1	B	207	1570	990	266	308	6	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	expression tag	UNP Q8NHL6-2
A	423	GLY	-	expression tag	UNP Q8NHL6-2
A	424	GLY	-	expression tag	UNP Q8NHL6-2
A	425	LEU	-	expression tag	UNP Q8NHL6-2
A	426	GLU	-	expression tag	UNP Q8NHL6-2
A	427	VAL	-	expression tag	UNP Q8NHL6-2
A	428	LEU	-	expression tag	UNP Q8NHL6-2
A	429	PHE	-	expression tag	UNP Q8NHL6-2
A	430	GLN	-	expression tag	UNP Q8NHL6-2
A	431	GLY	-	expression tag	UNP Q8NHL6-2
A	432	PRO	-	expression tag	UNP Q8NHL6-2
A	433	GLY	-	expression tag	UNP Q8NHL6-2
A	434	GLY	-	expression tag	UNP Q8NHL6-2
A	435	SER	-	expression tag	UNP Q8NHL6-2
A	436	ALA	-	expression tag	UNP Q8NHL6-2
A	437	TRP	-	expression tag	UNP Q8NHL6-2
A	438	SER	-	expression tag	UNP Q8NHL6-2
A	439	HIS	-	expression tag	UNP Q8NHL6-2
A	440	PRO	-	expression tag	UNP Q8NHL6-2
A	441	GLN	-	expression tag	UNP Q8NHL6-2
A	442	PHE	-	expression tag	UNP Q8NHL6-2
A	443	GLU	-	expression tag	UNP Q8NHL6-2
A	444	LYS	-	expression tag	UNP Q8NHL6-2
A	445	GLY	-	expression tag	UNP Q8NHL6-2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	GLY	-	expression tag	UNP Q8NHL6-2
A	447	HIS	-	expression tag	UNP Q8NHL6-2
A	448	HIS	-	expression tag	UNP Q8NHL6-2
A	449	HIS	-	expression tag	UNP Q8NHL6-2
A	450	HIS	-	expression tag	UNP Q8NHL6-2
A	451	HIS	-	expression tag	UNP Q8NHL6-2
A	452	HIS	-	expression tag	UNP Q8NHL6-2
A	453	HIS	-	expression tag	UNP Q8NHL6-2
A	454	HIS	-	expression tag	UNP Q8NHL6-2
B	422	GLY	-	expression tag	UNP Q8NHL6-2
B	423	GLY	-	expression tag	UNP Q8NHL6-2
B	424	GLY	-	expression tag	UNP Q8NHL6-2
B	425	LEU	-	expression tag	UNP Q8NHL6-2
B	426	GLU	-	expression tag	UNP Q8NHL6-2
B	427	VAL	-	expression tag	UNP Q8NHL6-2
B	428	LEU	-	expression tag	UNP Q8NHL6-2
B	429	PHE	-	expression tag	UNP Q8NHL6-2
B	430	GLN	-	expression tag	UNP Q8NHL6-2
B	431	GLY	-	expression tag	UNP Q8NHL6-2
B	432	PRO	-	expression tag	UNP Q8NHL6-2
B	433	GLY	-	expression tag	UNP Q8NHL6-2
B	434	GLY	-	expression tag	UNP Q8NHL6-2
B	435	SER	-	expression tag	UNP Q8NHL6-2
B	436	ALA	-	expression tag	UNP Q8NHL6-2
B	437	TRP	-	expression tag	UNP Q8NHL6-2
B	438	SER	-	expression tag	UNP Q8NHL6-2
B	439	HIS	-	expression tag	UNP Q8NHL6-2
B	440	PRO	-	expression tag	UNP Q8NHL6-2
B	441	GLN	-	expression tag	UNP Q8NHL6-2
B	442	PHE	-	expression tag	UNP Q8NHL6-2
B	443	GLU	-	expression tag	UNP Q8NHL6-2
B	444	LYS	-	expression tag	UNP Q8NHL6-2
B	445	GLY	-	expression tag	UNP Q8NHL6-2
B	446	GLY	-	expression tag	UNP Q8NHL6-2
B	447	HIS	-	expression tag	UNP Q8NHL6-2
B	448	HIS	-	expression tag	UNP Q8NHL6-2
B	449	HIS	-	expression tag	UNP Q8NHL6-2
B	450	HIS	-	expression tag	UNP Q8NHL6-2
B	451	HIS	-	expression tag	UNP Q8NHL6-2
B	452	HIS	-	expression tag	UNP Q8NHL6-2
B	453	HIS	-	expression tag	UNP Q8NHL6-2
B	454	HIS	-	expression tag	UNP Q8NHL6-2

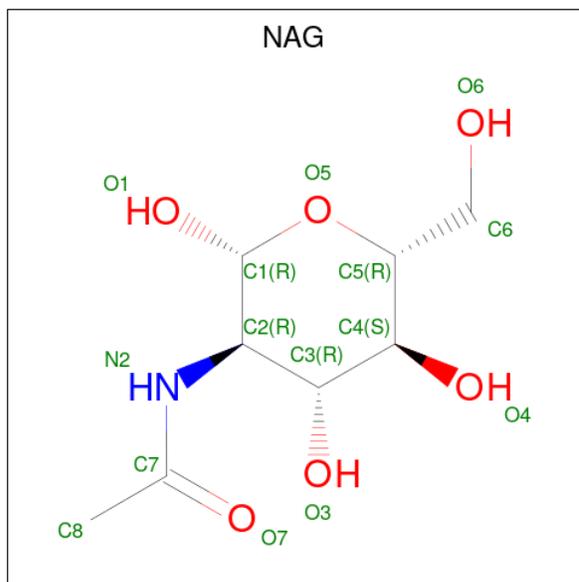
- Molecule 2 is a protein called Rifin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	125	Total 896	C 572	N 146	O 175	S 3	0	0	0
2	C	132	Total 940	C 599	N 153	O 185	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	238	GLN	ASN	conflict	UNP C0H5N9
E	323	GLN	ASN	conflict	UNP C0H5N9
C	238	GLN	ASN	conflict	UNP C0H5N9
C	323	GLN	ASN	conflict	UNP C0H5N9

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



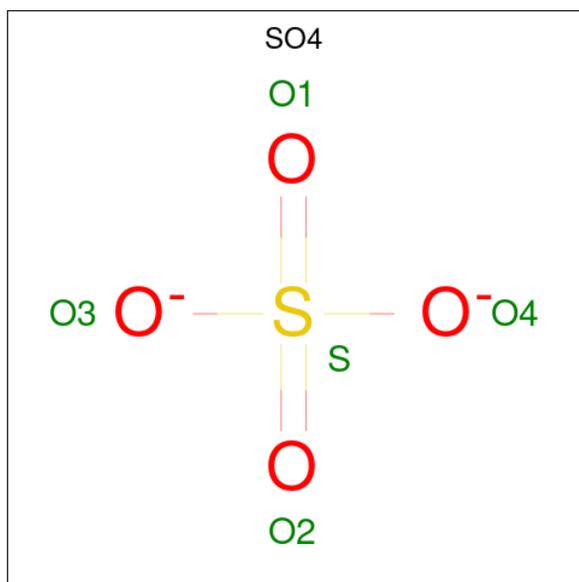
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

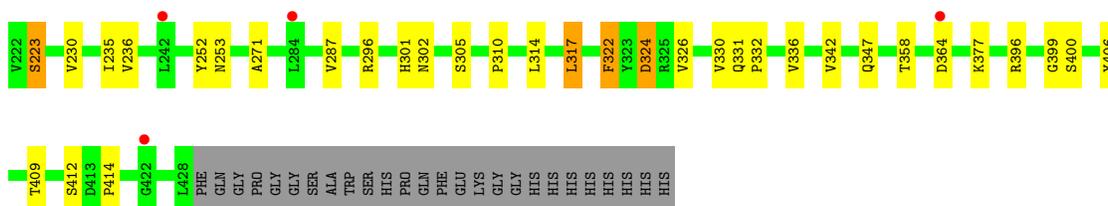
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	21	Total O 21 21	0	0
5	E	10	Total O 10 10	0	0
5	C	12	Total O 12 12	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

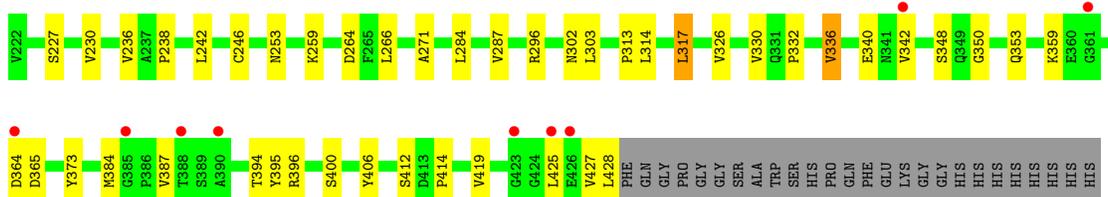
- Molecule 1: Isoform 2 of Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain A: 



- Molecule 1: Isoform 2 of Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain B: 



- Molecule 2: Rifin

Chain E: 



- Molecule 2: Rifin

Chain C: 



5311
5312
LYS
THR
LEU
ALA
VAL
GLU
THR
ALA
LYS
LYS
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.04Å 111.04Å 152.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 2.63 37.44 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.44-2.63) 99.2 (37.44-2.63)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.65Å)	Xtrriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.227 , 0.271 0.226 , 0.268	Depositor DCC
R_{free} test set	1415 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: SO4, NAG

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	0.39	0/1611	0.62	0/2195
1	B	0.33	0/1611	0.58	0/2195
2	C	0.37	0/956	0.60	2/1297 (0.2%)
2	E	0.33	0/912	0.57	1/1236 (0.1%)
All	All	0.36	0/5090	0.60	3/6923 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	215	LYS	CA-CB-CG	8.29	131.63	113.40
2	E	190	PRO	CA-N-CD	-7.94	100.38	111.50
2	C	215	LYS	CB-CG-CD	5.21	125.15	111.60

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	1570	0	1506	20	0
1	B	1570	0	1506	25	0
2	C	940	0	956	16	0
2	E	896	0	912	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	39	1	0
3	B	42	0	39	1	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	E	5	0	0	0	0
5	A	12	0	0	0	0
5	B	21	0	0	2	0
5	C	12	0	0	2	0
5	E	10	0	0	1	0
All	All	5150	0	4958	73	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 7.

All (73) 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:253:ASN:ND2	1:A:301:HIS:O	2.14	0.79
2:E:280:LYS:O	5:E:501:HOH:O	1.98	0.79
1:A:347:GLN:OE1	1:A:377:LYS:NZ	2.19	0.76
2:E:215:LYS:HA	2:E:218:ILE:HG22	1.68	0.75
1:B:236:VAL:HG11	1:B:242:LEU:HD21	1.69	0.74
2:C:203:LYS:O	5:C:501:HOH:O	2.06	0.74
2:E:197:ILE:HD11	2:E:218:ILE:HG21	1.68	0.73
1:A:230:VAL:HB	1:A:314:LEU:HD21	1.71	0.73
1:B:230:VAL:HB	1:B:314:LEU:HD21	1.72	0.71
2:C:234:TYR:HA	2:C:239:VAL:HG13	1.73	0.71
2:E:186:ALA:O	2:E:190:PRO:HD2	1.93	0.69
1:B:359:LYS:HD2	1:B:395:TYR:CZ	2.29	0.68
1:B:259:LYS:HB2	1:B:266:LEU:HD11	1.80	0.63
2:C:219:ASP:OD2	2:C:221:THR:OG1	2.17	0.62
2:E:227:SER:O	2:E:231:THR:HG23	2.00	0.61
1:A:326:VAL:HG23	1:A:412:SER:HB3	1.83	0.60
1:B:330:VAL:HG12	1:B:332:PRO:HD2	1.84	0.60
1:B:264:ASP:O	5:B:601:HOH:O	2.17	0.59
1:A:317:LEU:HD23	1:A:406:TYR:HA	1.85	0.57
2:C:229:ILE:O	2:C:233:ILE:HG13	2.05	0.56
2:E:225:ASP:OD2	2:E:228:TYR:N	2.34	0.55
2:C:201:LYS:HA	2:C:206:ILE:HB	1.87	0.55
1:A:330:VAL:HG12	1:A:332:PRO:HG2	1.89	0.55
2:C:214:LEU:O	2:C:218:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:NAG:H81	2:E:275:GLY:HA2	1.89	0.54
1:B:303:LEU:HD13	2:C:268:ASP:HB2	1.89	0.54
1:B:336:VAL:HG21	1:B:342:VAL:HG12	1.90	0.54
1:B:242:LEU:HB2	1:B:284:LEU:HB2	1.91	0.53
1:B:340:GLU:O	1:B:387:VAL:HG23	2.09	0.53
1:B:227:SER:O	1:B:246:CYS:HA	2.08	0.52
2:C:227:SER:O	2:C:231:THR:HG23	2.10	0.52
2:E:217:VAL:HG21	2:E:236:LYS:HE2	1.93	0.50
1:A:324:ASP:N	1:A:324:ASP:OD1	2.45	0.49
2:E:265:SER:O	2:E:269:LYS:HG3	2.12	0.49
1:B:236:VAL:CG1	1:B:242:LEU:HD21	2.41	0.49
1:B:342:VAL:HG23	1:B:384:MET:HB2	1.94	0.49
2:C:212:GLU:O	2:C:215:LYS:HB3	2.13	0.49
1:A:322:PHE:HD2	1:A:409:THR:HG22	1.78	0.49
1:A:223:SER:HB2	1:A:252:TYR:OH	2.12	0.48
1:A:336:VAL:HG11	1:A:342:VAL:HG22	1.94	0.48
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.64	0.48
1:A:399:GLY:O	1:A:409:THR:HG23	2.14	0.48
1:B:427:VAL:O	1:B:428:LEU:C	2.51	0.48
2:C:184:GLY:HA2	2:C:309:VAL:CG2	2.44	0.47
1:B:317:LEU:HD23	1:B:406:TYR:HA	1.96	0.47
1:B:353:GLN:NE2	5:B:604:HOH:O	2.47	0.46
1:B:348:SER:OG	1:B:350:GLY:O	2.33	0.46
2:E:193:ILE:HD13	2:E:219:ASP:HA	1.97	0.46
1:B:253:ASN:HA	1:B:271:ALA:O	2.16	0.46
2:C:215:LYS:O	2:C:216:SER:OG	2.22	0.46
1:B:326:VAL:HG23	1:B:412:SER:HB3	1.98	0.46
2:E:186:ALA:O	2:E:190:PRO:CD	2.64	0.45
2:E:269:LYS:HE2	2:E:269:LYS:HB2	1.78	0.45
1:A:331:GLN:N	1:A:332:PRO:HD2	2.31	0.45
1:B:296:ARG:NH1	1:B:313:PRO:HG3	2.31	0.45
3:B:501:NAG:H83	3:B:501:NAG:H3	1.98	0.45
2:E:192:ALA:O	2:E:196:VAL:HG22	2.17	0.45
1:A:236:VAL:HG13	1:A:287:VAL:HG21	1.99	0.44
1:B:396:ARG:CZ	1:B:414:PRO:HG3	2.47	0.44
2:C:208:THR:O	2:C:211:GLY:N	2.50	0.44
1:B:238:PRO:HA	1:B:287:VAL:HG23	2.00	0.43
2:C:214:LEU:O	2:C:217:VAL:HG22	2.18	0.43
1:B:303:LEU:HD21	2:C:264:CYS:HB3	1.99	0.43
1:A:377:LYS:HE3	1:A:377:LYS:HB2	1.64	0.42
1:A:396:ARG:HE	1:A:414:PRO:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:THR:HG23	2:E:221:THR:O	2.18	0.42
2:C:278:LEU:HD11	2:C:283:LEU:HD13	2.00	0.41
1:A:253:ASN:HA	1:A:271:ALA:O	2.20	0.41
1:A:253:ASN:HD21	1:A:302:ASN:HA	1.86	0.41
1:A:235:ILE:HD12	1:A:358:THR:HG21	2.03	0.41
1:A:296:ARG:HD3	1:A:310:PRO:HB2	2.02	0.41
2:C:223:TYR:OH	5:C:502:HOH:O	2.19	0.40
1:A:310:PRO:HD2	1:B:373:TYR:CZ	2.55	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	205/233 (88%)	202 (98%)	3 (2%)	0	100	100
1	B	205/233 (88%)	202 (98%)	3 (2%)	0	100	100
2	C	130/151 (86%)	126 (97%)	4 (3%)	0	100	100
2	E	123/151 (82%)	122 (99%)	1 (1%)	0	100	100
All	All	663/768 (86%)	652 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	170/190 (90%)	163 (96%)	7 (4%)	30	47
1	B	170/190 (90%)	161 (95%)	9 (5%)	22	36
2	C	97/111 (87%)	93 (96%)	4 (4%)	30	47
2	E	93/111 (84%)	89 (96%)	4 (4%)	29	45
All	All	530/602 (88%)	506 (96%)	24 (4%)	27	42

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	305	SER
1	A	317	LEU
1	A	322	PHE
1	A	324	ASP
1	A	364	ASP
1	A	400	SER
1	B	302	ASN
1	B	317	LEU
1	B	336	VAL
1	B	364	ASP
1	B	365	ASP
1	B	394	THR
1	B	400	SER
1	B	419	VAL
1	B	425	LEU
2	E	190	PRO
2	E	219	ASP
2	E	234	TYR
2	E	289	LYS
2	C	227	SER
2	C	279	ASP
2	C	281	SER
2	C	300	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	B	301	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
4	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	NAG	A	502	1	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	A	503	1	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	B	501	1	14,14,15	1.01	1 (7%)	17,19,21	1.80	3 (17%)
4	SO4	B	505	-	4,4,4	0.13	0	6,6,6	0.05	0
3	NAG	B	502	1	14,14,15	0.48	0	17,19,21	0.62	1 (5%)
4	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	401	-	4,4,4	0.15	0	6,6,6	0.05	0
3	NAG	B	503	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	A	501	1	14,14,15	0.28	0	17,19,21	0.43	0
4	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.04	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
3	NAG	A	502	1	-	3/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	5/6/23/26	0/1/1/1
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	B	503	1	-	3/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAG	O5-C1	3.48	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C1-O5-C5	5.22	119.26	112.19
3	B	501	NAG	C2-N2-C7	4.33	129.07	122.90
3	B	502	NAG	C1-O5-C5	2.10	115.03	112.19
3	B	501	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C4-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	B	501	NAG	C8-C7-N2-C2
3	B	501	NAG	O7-C7-N2-C2
3	B	503	NAG	C8-C7-N2-C2
3	B	503	NAG	O7-C7-N2-C2
3	A	502	NAG	C1-C2-N2-C7
3	B	503	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C3-C2-N2-C7
3	B	501	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	1	0
3	B	501	NAG	1	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	207/233 (88%)	-0.03	4 (1%) 66 64	30, 59, 89, 110	0
1	B	207/233 (88%)	0.25	9 (4%) 35 31	30, 57, 97, 112	0
2	C	132/151 (87%)	0.14	3 (2%) 60 57	39, 60, 91, 116	0
2	E	125/151 (82%)	0.24	11 (8%) 10 7	43, 61, 125, 150	0
All	All	671/768 (87%)	0.14	27 (4%) 38 35	30, 59, 98, 150	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	187	ALA	6.9
2	E	308	MET	6.6
2	E	307	ALA	6.2
2	E	304	ALA	5.3
2	E	186	ALA	5.0
2	E	184	GLY	4.8
2	E	306	ALA	4.3
2	E	303	LYS	4.3
1	B	388	THR	3.4
2	E	305	LYS	3.3
2	E	185	GLU	3.2
1	B	425	LEU	3.0
1	B	390	ALA	2.8
1	A	284	LEU	2.8
1	B	385	GLY	2.7
1	B	364	ASP	2.7
1	A	422	GLY	2.5
2	C	310	ALA	2.4
1	B	426	GLU	2.3
1	B	361	GLY	2.3
2	C	227	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	311	SER	2.2
1	A	242	LEU	2.2
1	B	423	GLY	2.2
1	A	364	ASP	2.1
2	E	188	ARG	2.1
1	B	342	VAL	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 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, 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
4	SO4	B	506	5/5	0.60	0.34	118,127,145,160	0
3	NAG	B	502	14/15	0.70	0.27	102,114,129,131	0
4	SO4	C	401	5/5	0.76	0.24	105,117,138,139	0
4	SO4	C	403	5/5	0.79	0.28	98,102,139,161	0
3	NAG	A	503	14/15	0.83	0.28	85,93,108,109	0
3	NAG	A	501	14/15	0.86	0.30	80,91,101,104	0
3	NAG	B	503	14/15	0.87	0.22	79,95,116,117	0
3	NAG	A	502	14/15	0.87	0.30	90,104,114,116	0
3	NAG	B	501	14/15	0.89	0.16	67,94,102,109	0
4	SO4	B	505	5/5	0.91	0.13	75,81,95,109	0
4	SO4	C	402	5/5	0.92	0.17	107,131,141,147	0
4	SO4	E	401	5/5	0.94	0.17	75,93,110,117	0
4	SO4	B	504	5/5	0.97	0.11	58,79,81,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.