



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:33 AM UTC

PDB ID : 7KFK / pdb_00007kfk
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 : 4-5-2 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

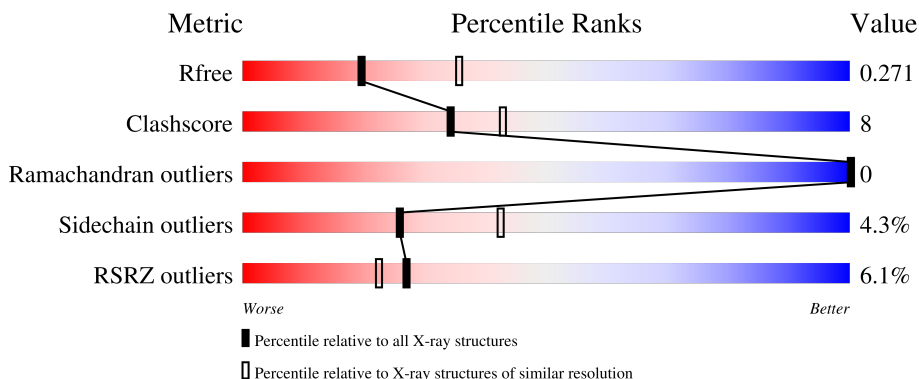
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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	6% 71% 16% • 11%
1	B	233	6% 70% 18% 11%
2	C	151	% 69% 17% • 13%
2	E	151	7% 69% 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
1	A	207	Total	C	N	O	S	0	0	0
			1570	990	266	308	6			
1	B	207	Total	C	N	O	S	0	0	0
			1570	990	266	308	6			

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

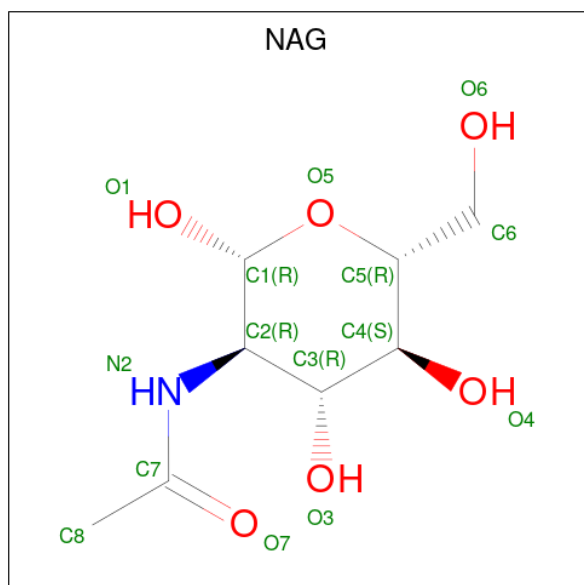
- Molecule 2 is a protein called Rifin.

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

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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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 (CCD ID: 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		

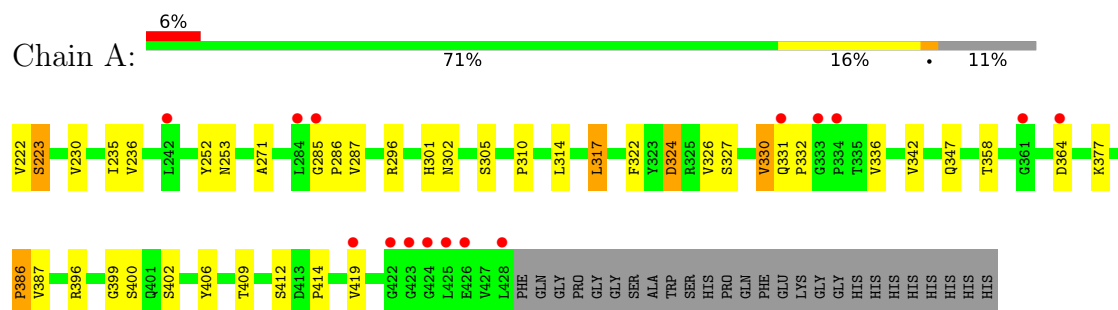
- Molecule 5 is water.

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

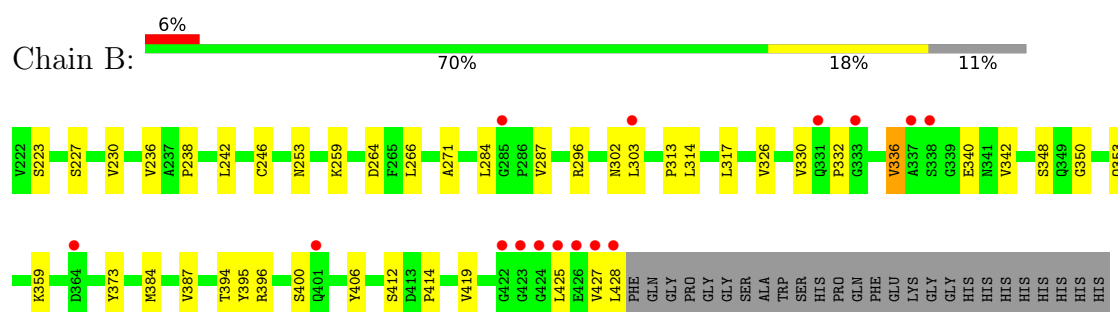
3 Residue-property plots [i](#)

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.

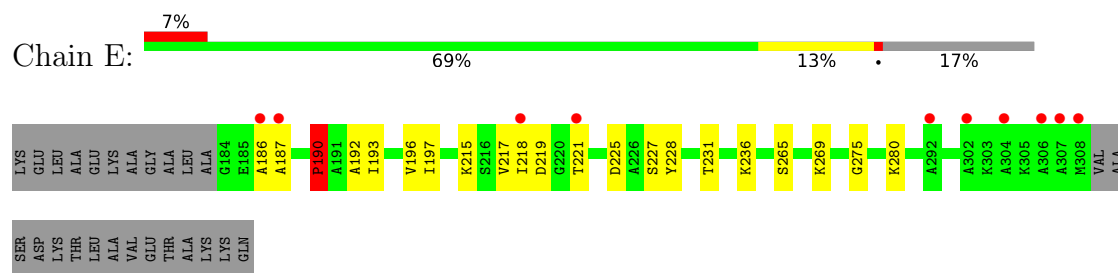
- Molecule 1: Isoform 2 of Leukocyte immunoglobulin-like receptor subfamily B member 1



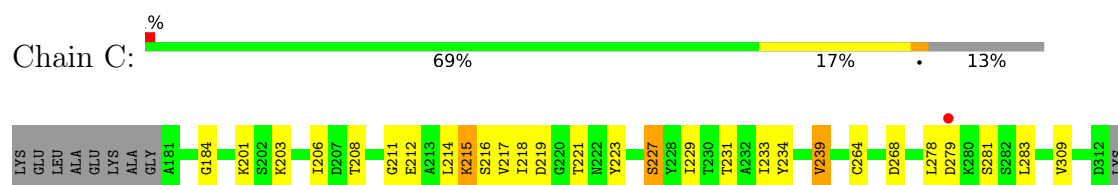
- Molecule 1: Isoform 2 of Leukocyte immunoglobulin-like receptor subfamily B member 1



- Molecule 2: Rifin



- Molecule 2: Rifin



THR
LEU
ALA
VAL
GLU
THR
ALA
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) 99.1 (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)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.227 , 0.271 0.231 , 0.271	Depositor DCC
R_{free} test set	1415 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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	0.47	1/1611 (0.1%)	0.71	0/2195
1	B	0.35	0/1611	0.62	0/2195
2	C	0.37	0/956	0.65	2/1297 (0.2%)
2	E	0.34	0/912	0.65	1/1236 (0.1%)
All	All	0.39	1/5090 (0.0%)	0.66	3/6923 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	PRO	C-O	-5.11	1.17	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	215	LYS	CA-CB-CG	8.77	131.63	114.10
2	E	190	PRO	CA-N-CD	-8.30	100.38	112.00
2	C	215	LYS	CB-CG-CD	6.02	125.15	111.30

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	22	0
1	B	1570	0	1506	25	0
2	C	940	0	956	16	0
2	E	896	0	912	15	0
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	76	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 8.

All (76) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:427:VAL:O	1:B:428:LEU:C	2.51	0.52
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
2:C:215:LYS:O	2:C:216:SER:OG	2.22	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
2:C:223:TYR:OH	5:C:502:HOH:O	2.19	0.48
1:A:399:GLY:O	1:A:409:THR:HG23	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:186:ALA:O	2:E:187:ALA:C	2.60	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
2:E:221:THR:HG23	2:E:221:THR:O	2.18	0.42
1:A:285:GLY:O	1:A:286:PRO:C	2.63	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
1:A:386:PRO:O	1:A:387:VAL:C	2.61	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 ⓘ

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%)	159 (94%)	11 (6%)	15	26
1	B	170/190 (90%)	163 (96%)	7 (4%)	27	44
2	C	97/111 (87%)	93 (96%)	4 (4%)	27	44
2	E	93/111 (84%)	92 (99%)	1 (1%)	65	79
All	All	530/602 (88%)	507 (96%)	23 (4%)	26	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	VAL
1	A	223	SER
1	A	305	SER
1	A	317	LEU
1	A	324	ASP
1	A	327	SER
1	A	330	VAL
1	A	364	ASP
1	A	400	SER
1	A	402	SER
1	A	419	VAL
1	B	223	SER
1	B	302	ASN
1	B	336	VAL
1	B	394	THR
1	B	400	SER
1	B	419	VAL
1	B	425	LEU
2	E	190	PRO
2	C	227	SER
2	C	239	VAL
2	C	279	ASP
2	C	281	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	321	GLN
1	A	379	GLN
1	B	301	HIS
2	C	276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	NAG	B	502	1	14,14,15	0.50	0	17,19,21	0.63	1 (5%)
3	NAG	A	503	1	14,14,15	0.24	0	17,19,21	0.38	0
4	SO4	B	505	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	403	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	504	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	C	402	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	501	1	14,14,15	0.99	1 (7%)	17,19,21	1.86	3 (17%)
4	SO4	E	401	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	B	506	-	4,4,4	0.24	0	6,6,6	0.09	0
3	NAG	A	501	1	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	B	503	1	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	A	502	1	14,14,15	0.37	0	17,19,21	0.41	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	B	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	6/6/23/26	0/1/1/1
3	NAG	A	501	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	502	1	-	2/6/23/26	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	3.32	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	5.28	119.26	112.19
3	B	501	NAG	C2-N2-C7	4.60	129.07	122.90
3	B	501	NAG	C1-C2-N2	2.20	113.91	110.43
3	B	502	NAG	C1-O5-C5	2.12	115.03	112.19

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

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Mol	Chain	Res	Type	Atoms
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	B	503	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	B	501	NAG	C1-C2-N2-C7
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%)	0.43	15 (7%) 21 17	30, 59, 89, 110	0
1	B	207/233 (88%)	0.48	15 (7%) 21 17	30, 57, 97, 112	0
2	C	132/151 (87%)	0.37	1 (0%) 82 80	39, 60, 91, 116	0
2	E	125/151 (82%)	0.43	10 (8%) 18 15	43, 61, 125, 150	0
All	All	671/768 (87%)	0.43	41 (6%) 27 22	30, 59, 98, 150	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	LEU	5.4
1	A	426	GLU	5.2
1	A	284	LEU	4.6
2	E	186	ALA	4.5
1	A	425	LEU	4.5
1	B	424	GLY	4.4
1	A	428	LEU	4.1
1	A	422	GLY	4.1
1	B	426	GLU	4.0
1	B	285	GLY	4.0
1	B	401	GLN	3.6
2	E	306	ALA	3.5
2	E	221	THR	3.2
1	B	423	GLY	3.2
1	A	242	LEU	3.1
1	B	331	GLN	3.1
1	A	424	GLY	3.0
2	E	308	MET	2.9
2	E	304	ALA	2.8
1	B	422	GLY	2.8
1	A	419	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	331	GLN	2.7
1	A	423	GLY	2.6
1	B	425	LEU	2.5
1	A	361	GLY	2.5
1	B	338	SER	2.5
1	A	364	ASP	2.5
2	E	187	ALA	2.5
2	E	302	ALA	2.3
1	B	364	ASP	2.3
1	B	337	ALA	2.3
1	B	333	GLY	2.3
1	A	333	GLY	2.2
2	E	218	ILE	2.2
2	C	279	ASP	2.2
2	E	307	ALA	2.2
1	B	427	VAL	2.2
2	E	292	ALA	2.1
1	B	303	LEU	2.0
1	A	285	GLY	2.0
1	A	334	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	401	5/5	0.53	0.10	105,117,138,139	0
4	SO4	C	403	5/5	0.53	0.11	98,102,139,161	0
4	SO4	B	506	5/5	0.57	0.11	118,127,145,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	502	14/15	0.59	0.15	102,114,129,131	0
3	NAG	B	503	14/15	0.62	0.14	79,95,116,117	0
3	NAG	A	502	14/15	0.63	0.14	90,104,114,116	0
3	NAG	A	503	14/15	0.71	0.14	85,93,108,109	0
4	SO4	C	402	5/5	0.77	0.07	107,131,141,147	0
3	NAG	A	501	14/15	0.81	0.12	80,91,101,104	0
3	NAG	B	501	14/15	0.81	0.12	67,94,102,109	0
4	SO4	E	401	5/5	0.85	0.09	75,93,110,117	0
4	SO4	B	505	5/5	0.91	0.11	75,81,95,109	0
4	SO4	B	504	5/5	0.91	0.14	58,79,81,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.