



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:30 AM UTC

PDB ID : 6RUU / pdb_00006ruu
Title : Pseudokinase domain of human IRAK3
Authors : Lange, S.M.; Kulathu, Y.; Cohen, P.
Deposited on : 2019-05-29
Resolution : 2.95 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

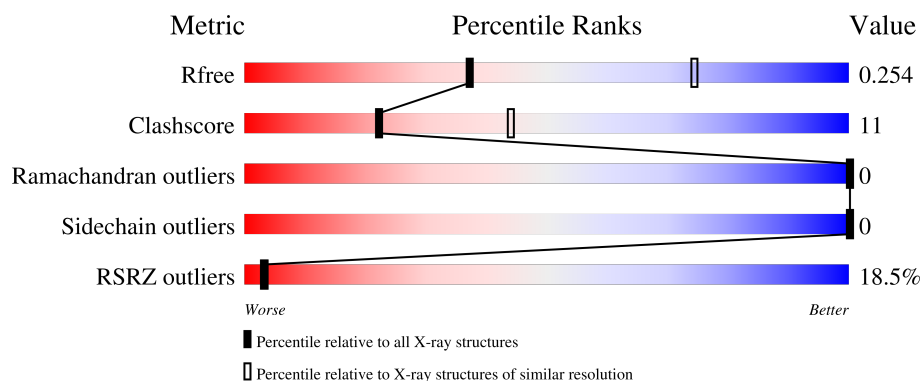
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	315	13% 72% 18% 10%
1	B	315	25% 67% 24% 9%
1	C	315	10% 60% 18% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	508	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6252 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 Interleukin-1 receptor-associated kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2223	1438	376	392	17			
1	B	286	Total	C	N	O	S	0	0	0
			2102	1356	351	379	16			
1	C	245	Total	C	N	O	S	0	0	0
			1861	1205	311	330	15			

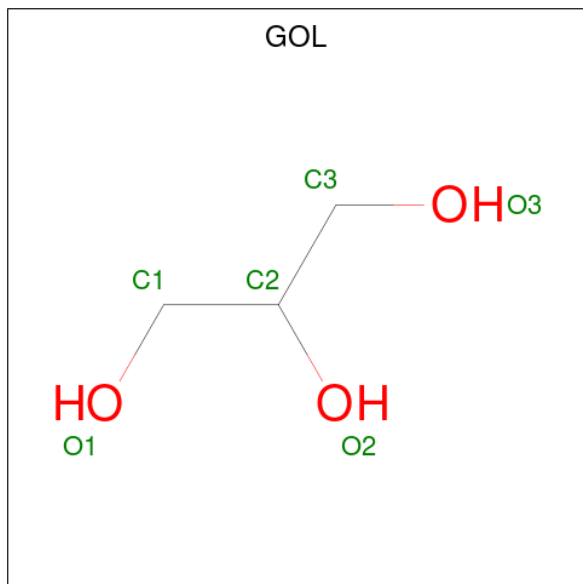
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	GLY	-	expression tag	UNP Q9Y616
A	141	PRO	-	expression tag	UNP Q9Y616
A	142	LEU	-	expression tag	UNP Q9Y616
A	143	GLY	-	expression tag	UNP Q9Y616
A	144	SER	-	expression tag	UNP Q9Y616
A	147	VAL	ILE	variant	UNP Q9Y616
B	140	GLY	-	expression tag	UNP Q9Y616
B	141	PRO	-	expression tag	UNP Q9Y616
B	142	LEU	-	expression tag	UNP Q9Y616
B	143	GLY	-	expression tag	UNP Q9Y616
B	144	SER	-	expression tag	UNP Q9Y616
B	147	VAL	ILE	variant	UNP Q9Y616
C	140	GLY	-	expression tag	UNP Q9Y616
C	141	PRO	-	expression tag	UNP Q9Y616
C	142	LEU	-	expression tag	UNP Q9Y616
C	143	GLY	-	expression tag	UNP Q9Y616
C	144	SER	-	expression tag	UNP Q9Y616
C	147	VAL	ILE	variant	UNP Q9Y616

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

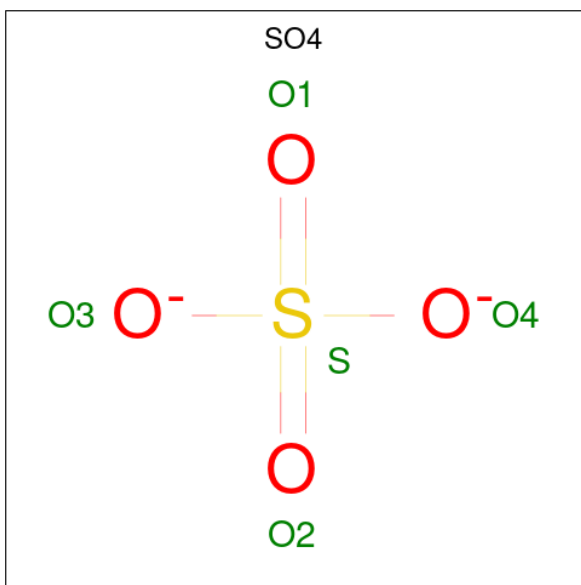
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Hg 2 2	0	0
2	B	1	Total Hg 1 1	0	0
2	C	5	Total Hg 5 5	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

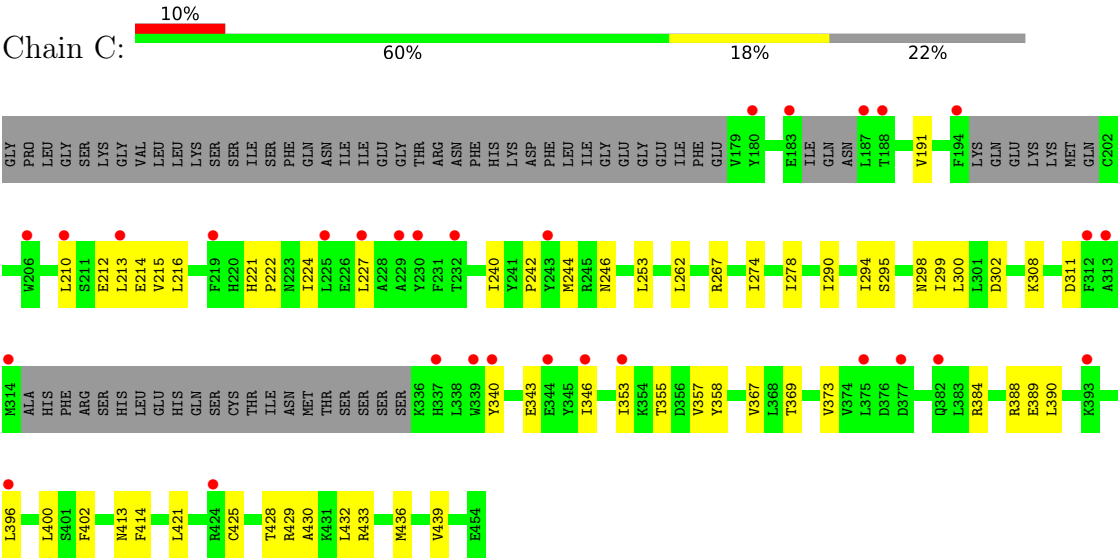


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	53.55Å 167.16Å 179.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.95 48.65 – 2.95	Depositor EDS
% Data completeness (in resolution range)	61.6 (48.65-2.95) 57.2 (48.65-2.95)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.260 0.229 , 0.254	Depositor DCC
R_{free} test set	1119 reflections (3.21%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 92.9	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	0.90	EDS
Total number of atoms	6252	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, GOL, HG

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	0.15	0/2272	0.38	0/3076
1	B	0.12	0/2147	0.33	0/2927
1	C	0.15	0/1902	0.37	0/2588
All	All	0.14	0/6321	0.36	0/8591

There are no bond length outliers.

There are no bond angle outliers.

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	2223	0	2162	45	0
1	B	2102	0	1935	48	0
1	C	1861	0	1786	43	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	5	0	0	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
4	A	20	0	0	0	0
4	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	10	0	0	3	0
All	All	6252	0	5907	129	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 11.

All (129) 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:B:162:THR:HG23	1:B:165:PHE:H	1.43	0.83
1:B:252:ARG:HE	1:B:259:THR:HG21	1.48	0.79
1:B:208:ARG:HE	1:B:314:MET:HE3	1.48	0.79
1:C:191:VAL:HG12	1:C:240:ILE:HG22	1.65	0.78
1:C:430:ALA:HA	1:C:433:ARG:HE	1.49	0.76
1:A:362:ILE:HA	1:A:365:MET:HE3	1.67	0.76
1:A:295:SER:HA	1:A:340:TYR:HE2	1.49	0.75
1:B:179:VAL:HG12	1:B:192:LYS:HG2	1.67	0.74
1:A:381:ILE:HD11	1:C:389:GLU:HG3	1.71	0.71
1:B:263:PRO:HD2	1:B:266:ILE:HD12	1.73	0.70
1:A:295:SER:HA	1:A:340:TYR:CE2	2.27	0.70
1:B:228:ALA:HB3	1:B:240:ILE:HG13	1.75	0.69
1:A:246:ASN:ND2	1:A:302:ASP:O	2.25	0.68
1:C:357:VAL:HG22	1:C:436:MET:HE2	1.77	0.67
1:A:357:VAL:HG12	1:A:436:MET:HE2	1.77	0.66
1:A:244:MET:HE3	1:A:308:LYS:HG3	1.75	0.66
1:C:246:ASN:ND2	1:C:302:ASP:O	2.29	0.66
1:A:162:THR:HG23	1:A:165:PHE:H	1.59	0.66
1:A:163:ARG:HD3	1:A:169:PHE:HE2	1.60	0.66
1:B:171:ILE:HB	1:B:179:VAL:HG23	1.77	0.65
1:C:221:HIS:CD2	1:C:222:PRO:HD2	2.32	0.64
1:A:402:PHE:HE2	1:C:390:LEU:HD23	1.63	0.63
1:A:427:ALA:O	1:A:433:ARG:NH1	2.32	0.62
1:C:421:LEU:HD21	1:C:439:VAL:HG23	1.82	0.61
1:A:191:VAL:HG12	1:A:240:ILE:HG22	1.82	0.61
1:A:394:ARG:NH2	1:C:369:THR:O	2.34	0.60
1:B:270:ILE:HG22	1:B:307:PRO:HD3	1.83	0.60
1:C:430:ALA:HA	1:C:433:ARG:NE	2.18	0.59
1:A:163:ARG:HD3	1:A:169:PHE:CE2	2.38	0.59
1:B:410:CYS:SG	1:B:415:SER:OG	2.61	0.58
1:A:293:SER:OG	1:A:311:ASP:O	2.22	0.58
1:B:274:ILE:HD11	1:B:307:PRO:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HB3	1:A:262:LEU:HD11	1.86	0.58
1:B:224:ILE:HD11	1:B:281:LEU:HD21	1.85	0.58
1:A:237:PHE:CE2	1:B:286:PRO:HG3	2.40	0.57
1:B:213:LEU:HD12	1:B:239:LEU:HD21	1.88	0.56
1:A:270:ILE:HG23	1:A:307:PRO:HB3	1.89	0.55
1:B:388:ARG:HH22	1:B:428:THR:HG23	1.72	0.54
1:B:173:GLU:HA	1:B:178:GLU:HA	1.89	0.54
1:B:191:VAL:HG12	1:B:240:ILE:HG22	1.90	0.54
1:A:402:PHE:CE2	1:C:390:LEU:HD23	2.43	0.54
1:A:248:THR:HG23	1:A:251:ASP:H	1.73	0.53
1:B:208:ARG:HB3	1:B:313:ALA:HB1	1.89	0.52
1:B:158:ILE:O	1:B:162:THR:HG22	2.09	0.52
1:B:437:ASP:OD1	1:B:438:GLU:N	2.42	0.52
1:C:253:LEU:HD21	1:C:367:VAL:HG23	1.91	0.52
1:C:358:TYR:HB2	1:C:433:ARG:NH2	2.25	0.52
1:A:225:LEU:HD22	1:A:300:LEU:HD12	1.92	0.52
1:B:282:HIS:HD2	1:B:353:ILE:HG23	1.74	0.51
1:B:387:LEU:HD23	1:B:390:LEU:HD12	1.91	0.51
1:A:281:LEU:HB3	1:A:289:VAL:HG13	1.92	0.51
1:A:344:GLU:OE2	1:A:433:ARG:NH2	2.43	0.51
1:C:295:SER:HA	1:C:340:TYR:CE2	2.44	0.51
1:B:271:LEU:HD11	1:B:364:ILE:HG12	1.93	0.51
1:A:183:GLU:HA	1:A:188:THR:HA	1.92	0.50
1:C:210:LEU:O	1:C:214:GLU:HG3	2.11	0.50
1:B:208:ARG:NH2	1:B:332:SER:O	2.41	0.50
1:A:188:THR:HG23	1:A:243:TYR:HB3	1.93	0.50
1:A:394:ARG:HG3	1:C:402:PHE:HA	1.93	0.50
1:A:224:ILE:HD11	1:A:281:LEU:HD11	1.94	0.49
1:A:267:ARG:NH2	1:A:404:ASP:OD2	2.45	0.49
1:C:295:SER:HA	1:C:340:TYR:HE2	1.77	0.49
1:B:244:MET:HG3	1:B:300:LEU:HB3	1.95	0.49
1:A:162:THR:HA	1:A:169:PHE:HD2	1.77	0.49
1:C:413:ASN:OD1	1:C:414:PHE:N	2.46	0.49
1:B:391:MET:HE1	1:B:423:GLY:HA3	1.95	0.49
1:C:221:HIS:HB3	1:C:224:ILE:HG12	1.93	0.48
1:C:242:PRO:HB2	1:C:244:MET:HE2	1.93	0.48
1:C:358:TYR:HA	1:C:425:CYS:O	2.13	0.48
1:B:314:MET:HE2	1:B:334:SER:HB2	1.95	0.48
1:C:244:MET:HE3	1:C:308:LYS:HG3	1.95	0.48
1:C:384:ARG:O	1:C:388:ARG:HG2	2.14	0.48
1:C:388:ARG:NH1	1:C:428:THR:HG23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HB3	1:A:262:LEU:CD1	2.43	0.48
1:C:212:GLU:OE1	1:C:311:ASP:HB3	2.13	0.48
1:B:278:ILE:HB	1:B:436:MET:HE2	1.95	0.48
1:A:177:PHE:CD2	1:A:192:LYS:HG2	2.50	0.47
1:C:340:TYR:CE1	1:C:373:VAL:HG21	2.49	0.47
1:B:216:LEU:HB3	1:B:227:LEU:HB2	1.97	0.47
1:C:278:ILE:HG21	1:C:294:ILE:HD12	1.95	0.47
1:B:357:VAL:HG12	1:B:436:MET:SD	2.55	0.47
1:B:248:THR:HG22	1:B:250:PHE:H	1.79	0.47
1:B:254:GLN:NE2	1:B:370:GLY:O	2.48	0.47
1:A:340:TYR:CE1	1:A:373:VAL:HG21	2.50	0.46
1:A:429:ARG:HG3	1:A:432:LEU:HD23	1.98	0.46
1:C:429:ARG:HG3	1:C:432:LEU:HD13	1.98	0.46
1:A:216:LEU:HD13	1:A:227:LEU:HB2	1.98	0.46
1:B:154:SER:OG	1:B:157:ASN:OD1	2.23	0.46
1:B:274:ILE:HG13	1:B:299:ILE:HD13	1.97	0.46
1:C:290:ILE:HG21	1:C:353:ILE:HA	1.98	0.46
1:C:300:LEU:HB2	1:C:308:LYS:HB2	1.98	0.45
1:B:274:ILE:CD1	1:B:307:PRO:HB2	2.46	0.45
1:C:210:LEU:O	1:C:214:GLU:N	2.45	0.45
1:C:388:ARG:NH2	4:C:508:SO4:O1	2.28	0.45
1:C:213:LEU:HD12	1:C:227:LEU:HD13	1.98	0.45
1:A:180:TYR:HB2	1:A:191:VAL:CG2	2.47	0.44
1:A:278:ILE:HG21	1:A:436:MET:HE3	1.99	0.44
1:B:248:THR:HG22	1:B:250:PHE:N	2.32	0.44
1:C:429:ARG:NE	4:C:508:SO4:O2	2.50	0.44
1:A:340:TYR:HE1	1:A:373:VAL:HG11	1.83	0.44
1:B:210:LEU:O	1:B:214:GLU:HG3	2.18	0.44
1:B:221:HIS:CG	1:B:222:PRO:HD2	2.52	0.44
1:A:302:ASP:OD1	1:A:306:GLN:N	2.42	0.44
1:B:203:LYS:O	1:B:207:LYS:HD3	2.17	0.44
1:C:262:LEU:HB2	1:C:267:ARG:HE	1.83	0.44
1:B:281:LEU:HD12	1:B:289:VAL:HG11	1.99	0.44
1:C:396:LEU:O	1:C:400:LEU:HG	2.17	0.43
1:B:345:TYR:CE1	1:B:351:LEU:HD12	2.54	0.43
1:C:215:VAL:HG13	1:C:216:LEU:HD12	2.00	0.43
1:C:343:GLU:HA	1:C:346:ILE:HG12	2.00	0.43
1:A:210:LEU:HD23	1:B:214:GLU:CD	2.43	0.42
1:A:170:LEU:HA	1:A:180:TYR:HA	2.01	0.42
1:A:368:LEU:HD21	1:A:418:LEU:HD22	2.00	0.42
1:B:310:THR:HG22	1:B:311:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:HA	1:A:307:PRO:HG3	2.02	0.42
1:B:172:GLY:O	1:B:179:VAL:N	2.52	0.42
1:B:190:ALA:HB2	1:B:243:TYR:HD1	1.83	0.42
1:B:216:LEU:HD13	1:B:227:LEU:HB2	2.02	0.42
1:A:252:ARG:HG3	1:A:301:LEU:HD12	2.02	0.42
1:A:291:CYS:HB2	1:A:294:ILE:HD11	2.02	0.42
1:B:369:THR:C	1:B:371:CYS:H	2.29	0.41
1:B:272:ILE:HG23	1:B:440:LEU:HD11	2.02	0.41
1:A:368:LEU:HD11	1:A:418:LEU:HB3	2.03	0.41
1:C:353:ILE:HD12	1:C:353:ILE:H	1.86	0.41
1:C:355:THR:O	1:C:358:TYR:HB3	2.20	0.41
1:C:428:THR:N	4:C:508:SO4:O4	2.54	0.41
1:C:298:ASN:ND2	1:C:311:ASP:O	2.54	0.40
1:B:293:SER:OG	1:B:311:ASP:O	2.40	0.40
1:C:274:ILE:HD13	1:C:299:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	277/315 (88%)	264 (95%)	13 (5%)	0	100	100
1	B	278/315 (88%)	268 (96%)	10 (4%)	0	100	100
1	C	237/315 (75%)	228 (96%)	9 (4%)	0	100	100
All	All	792/945 (84%)	760 (96%)	32 (4%)	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	233/284 (82%)	233 (100%)	0	100	100
1	B	204/284 (72%)	204 (100%)	0	100	100
1	C	191/284 (67%)	191 (100%)	0	100	100
All	All	628/852 (74%)	628 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	220	HIS
1	A	283	ASN
1	B	447	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	502	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	508	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	C	507	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	A	505	-	4,4,4	0.24	0	6,6,6	0.12	0
3	GOL	A	503	-	5,5,5	0.96	0	5,5,5	1.06	0
3	GOL	C	506	-	5,5,5	0.99	0	5,5,5	1.03	0
4	SO4	A	507	-	4,4,4	0.24	0	6,6,6	0.11	0
3	GOL	A	504	-	5,5,5	0.93	0	5,5,5	1.07	0
4	SO4	A	508	-	4,4,4	0.25	0	6,6,6	0.06	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	GOL	A	504	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	C	506	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	506	GOL	C1-C2-C3-O3
3	C	506	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	508	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/315 (90%)	0.99	41 (14%) 6 5	30, 69, 126, 171	0
1	B	286/315 (90%)	1.48	80 (27%) 1 1	83, 123, 167, 196	0
1	C	245/315 (77%)	0.86	30 (12%) 8 8	28, 60, 125, 150	0
All	All	816/945 (86%)	1.12	151 (18%) 3 3	28, 96, 150, 196	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	ALA	6.3
1	B	319	SER	5.2
1	A	237	PHE	4.9
1	C	230	TYR	4.9
1	A	376	ASP	4.9
1	B	394	ARG	4.8
1	B	360	PHE	4.6
1	B	264	TRP	4.5
1	C	219	PHE	4.4
1	A	327	THR	4.3
1	C	377	ASP	4.2
1	B	184	ILE	4.2
1	A	325	SER	4.2
1	C	213	LEU	4.0
1	B	289	VAL	4.0
1	B	415	SER	3.9
1	B	396	LEU	3.8
1	A	165	PHE	3.8
1	A	197	GLU	3.8
1	A	158	ILE	3.8
1	B	238	CYS	3.7
1	C	206	TRP	3.7
1	B	170	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	183	GLU	3.6
1	A	337	HIS	3.5
1	A	326	CYS	3.5
1	B	402	PHE	3.5
1	A	209	PHE	3.5
1	C	314	MET	3.5
1	B	421	LEU	3.5
1	B	353	ILE	3.5
1	A	346	ILE	3.4
1	C	183	GLU	3.4
1	A	201	GLN	3.4
1	B	169	PHE	3.4
1	B	351	LEU	3.4
1	B	168	ASP	3.4
1	B	373	VAL	3.3
1	B	218	LEU	3.3
1	B	452	PHE	3.3
1	A	202	CYS	3.3
1	A	231	PHE	3.2
1	B	291	CYS	3.2
1	B	274	ILE	3.2
1	B	412	ARG	3.1
1	C	337	HIS	3.1
1	B	191	VAL	3.0
1	B	305	PHE	3.0
1	B	357	VAL	3.0
1	A	171	ILE	3.0
1	B	178	GLU	3.0
1	B	195	LYS	3.0
1	B	414	PHE	3.0
1	B	188	THR	3.0
1	B	234	THR	3.0
1	B	317	PHE	3.0
1	A	153	ILE	2.9
1	B	278	ILE	2.9
1	C	243	TYR	2.9
1	B	446	THR	2.9
1	A	360	PHE	2.9
1	B	292	GLY	2.8
1	B	426	ALA	2.8
1	B	419	PHE	2.8
1	B	166	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	201	GLN	2.7
1	C	312	PHE	2.7
1	A	440	LEU	2.7
1	B	271	LEU	2.7
1	A	179	VAL	2.7
1	A	181	ARG	2.6
1	B	265	HIS	2.6
1	B	173	GLU	2.6
1	A	191	VAL	2.6
1	A	218	LEU	2.6
1	B	328	ILE	2.6
1	C	194	PHE	2.6
1	B	152	SER	2.6
1	B	339	TRP	2.5
1	B	338	LEU	2.5
1	B	386	LEU	2.5
1	C	225	LEU	2.5
1	C	340	TYR	2.5
1	C	339	TRP	2.5
1	B	190	ALA	2.5
1	B	267	ARG	2.5
1	A	381	ILE	2.5
1	B	420	CYS	2.5
1	B	375	LEU	2.4
1	C	227	LEU	2.4
1	A	345	TYR	2.4
1	B	189	TYR	2.4
1	C	187	LEU	2.4
1	B	428	THR	2.4
1	A	309	LEU	2.4
1	C	353	ILE	2.4
1	B	451	TYR	2.4
1	C	344	GLU	2.3
1	B	401	SER	2.3
1	B	204	LYS	2.3
1	B	233	GLU	2.3
1	B	442	THR	2.3
1	B	413	ASN	2.3
1	A	330	MET	2.3
1	A	213	LEU	2.3
1	B	253	LEU	2.3
1	B	403	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	176	ILE	2.3
1	B	381	ILE	2.3
1	B	258	ASP	2.3
1	B	364	ILE	2.3
1	B	369	THR	2.3
1	C	393	LYS	2.2
1	A	238	CYS	2.2
1	B	425	CYS	2.2
1	B	206	TRP	2.2
1	B	175	GLU	2.2
1	A	331	THR	2.2
1	C	396	LEU	2.2
1	B	450	LEU	2.2
1	C	424	ARG	2.2
1	A	206	TRP	2.2
1	B	371	CYS	2.2
1	A	448	ALA	2.2
1	B	424	ARG	2.1
1	C	188	THR	2.1
1	C	232	THR	2.1
1	C	346	ILE	2.1
1	C	382	GLN	2.1
1	A	329	ASN	2.1
1	B	203	LYS	2.1
1	B	193	LEU	2.1
1	A	214	GLU	2.1
1	B	202	CYS	2.1
1	A	396	LEU	2.1
1	A	235	GLU	2.1
1	B	380	HIS	2.1
1	B	312	PHE	2.1
1	A	236	LYS	2.0
1	A	288	SER	2.0
1	A	398	SER	2.0
1	B	387	LEU	2.0
1	A	174	GLY	2.0
1	B	192	LYS	2.0
1	C	210	LEU	2.0
1	C	375	LEU	2.0
1	A	384	ARG	2.0
1	B	329	ASN	2.0
1	C	313	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	241	TYR	2.0
1	C	180	TYR	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
3	GOL	A	503	6/6	0.54	0.18	90,97,102,108	0
4	SO4	B	503	5/5	0.71	0.10	125,135,143,145	0
4	SO4	B	502	5/5	0.72	0.15	82,97,104,120	0
4	SO4	A	508	5/5	0.73	0.10	130,137,144,151	0
3	GOL	A	504	6/6	0.75	0.16	73,75,77,85	0
2	HG	C	505	1/1	0.76	0.18	130,130,130,130	1
4	SO4	A	507	5/5	0.80	0.17	119,126,128,134	0
2	HG	C	501	1/1	0.81	0.11	78,78,78,78	1
3	GOL	C	506	6/6	0.84	0.19	66,86,93,94	0
4	SO4	C	507	5/5	0.90	0.08	69,77,96,103	0
2	HG	C	504	1/1	0.92	0.14	162,162,162,162	1
4	SO4	A	505	5/5	0.95	0.09	59,67,69,69	0
2	HG	A	502	1/1	0.95	0.14	73,73,73,73	1
4	SO4	A	506	5/5	0.96	0.08	62,67,71,73	0
4	SO4	C	508	5/5	0.96	0.04	54,62,67,75	0
2	HG	C	502	1/1	0.97	0.11	56,56,56,56	1
2	HG	C	503	1/1	0.97	0.10	114,114,114,114	0
2	HG	A	501	1/1	0.97	0.12	100,100,100,100	1
2	HG	B	501	1/1	0.98	0.04	74,74,74,74	1

6.5 Other polymers [i](#)

There are no such residues in this entry.