



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:01 PM UTC

PDB ID : 5LXG / pdb_00005lxg
Title : Revised crystal structure of the human adiponectin receptor 1 in an open conformation
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Deposited on : 2016-09-21
Resolution : 2.73 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

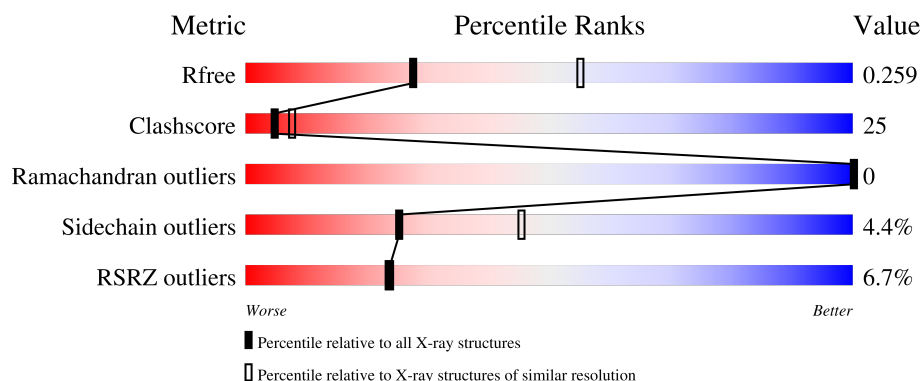
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	305	10% 53% 35% • 8%
2	H	119	2% 69% 28% •
3	L	107	77% 21% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4213 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 Adiponectin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	48	0	0
			2286	1530	374	367	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q96A54
A	-16	ASP	-	expression tag	UNP Q96A54
A	-15	TYR	-	expression tag	UNP Q96A54
A	-14	LYS	-	expression tag	UNP Q96A54
A	-13	ASP	-	expression tag	UNP Q96A54
A	-12	ASP	-	expression tag	UNP Q96A54
A	-11	ASP	-	expression tag	UNP Q96A54
A	-10	ASP	-	expression tag	UNP Q96A54
A	-9	LYS	-	expression tag	UNP Q96A54
A	-8	GLU	-	expression tag	UNP Q96A54
A	-7	ASN	-	expression tag	UNP Q96A54
A	-6	LEU	-	expression tag	UNP Q96A54
A	-5	TYR	-	expression tag	UNP Q96A54
A	-4	PHE	-	expression tag	UNP Q96A54
A	-3	GLN	-	expression tag	UNP Q96A54
A	-2	GLY	-	expression tag	UNP Q96A54
A	-1	GLY	-	expression tag	UNP Q96A54
A	0	SER	-	expression tag	UNP Q96A54

- Molecule 2 is a protein called V REGION HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			927	592	149	182	4			

- Molecule 3 is a protein called V REGION LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	107	Total	C	N	O	S	0	0	0
			820	517	137	163	3			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	H	29	Total	O	0	0
			29	29		
6	L	38	Total	O	0	0
			38	38		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.31Å 194.11Å 74.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.66 – 2.73 26.66 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.1 (26.66-2.73) 98.1 (26.66-2.73)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.225 , 0.234 0.237 , 0.259	Depositor DCC
R_{free} test set	891 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4213	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.78	3/2368 (0.1%)	1.46	12/3217 (0.4%)
2	H	0.60	0/951	1.03	3/1291 (0.2%)
3	L	0.55	0/840	0.91	0/1140
All	All	0.70	3/4159 (0.1%)	1.28	15/5648 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	MET	SD-CE	-9.15	1.56	1.79
1	A	300	MET	SD-CE	-6.34	1.63	1.79
1	A	233	GLN	C-N	5.10	1.40	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	MET	N-CA-C	-9.75	100.51	111.82
1	A	157	LEU	N-CA-C	-7.38	99.31	109.71
2	H	89	GLU	CB-CG-CD	5.91	122.64	112.60
1	A	302	TRP	CA-C-N	5.88	130.53	120.72
1	A	302	TRP	C-N-CA	5.88	130.53	120.72
1	A	168	GLN	CA-C-N	5.77	129.84	120.60
1	A	168	GLN	C-N-CA	5.77	129.84	120.60
1	A	256	ASP	CA-CB-CG	5.43	118.03	112.60
2	H	67	LYS	CG-CD-CE	-5.37	98.94	111.30
1	A	168	GLN	N-CA-C	-5.35	105.62	111.82
1	A	138	ILE	CA-C-N	5.30	127.38	120.28
1	A	138	ILE	C-N-CA	5.30	127.38	120.28
1	A	247	ILE	N-CA-C	-5.18	105.45	110.42
1	A	258	PHE	N-CA-C	5.09	116.58	108.79
2	H	61	ASN	N-CA-C	-5.07	103.35	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2286	0	2271	154	2
2	H	927	0	886	28	2
3	L	820	0	786	19	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
5	L	5	0	0	0	0
6	A	102	0	0	1	0
6	H	29	0	0	0	0
6	L	38	0	0	0	0
All	All	4213	0	3943	200	2

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 25.

All (200) 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:299:GLN:HB3	1:A:302:TRP:HD1	1.12	1.11
1:A:356:SER:O	1:A:359:GLN:HG2	1.51	1.11
1:A:299:GLN:NE2	1:A:357:ASN:HB2	1.67	1.09
1:A:310:TYR:HE1	1:A:347:ALA:CB	1.63	1.09
1:A:272:LEU:CD2	1:A:276:LEU:HD11	1.85	1.07
1:A:272:LEU:HD21	1:A:276:LEU:HD11	1.34	1.07
1:A:299:GLN:HE22	1:A:357:ASN:HB2	0.94	1.04
1:A:252:VAL:HG11	1:A:267:ARG:HA	1.41	1.03
1:A:278:GLY:O	1:A:282:THR:HG22	1.56	1.01
1:A:299:GLN:HB3	1:A:302:TRP:CD1	1.99	0.97
1:A:238:TYR:HE2	1:A:281:PRO:CA	1.77	0.96
1:A:310:TYR:CE1	1:A:347:ALA:CB	2.48	0.95
1:A:172:VAL:CG1	1:A:222:PRO:HA	1.96	0.95
1:A:310:TYR:HE1	1:A:347:ALA:HB3	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:MET:HE1	1:A:351:HIS:HD2	1.33	0.94
1:A:272:LEU:CD2	1:A:276:LEU:CD1	2.47	0.92
1:A:310:TYR:HE1	1:A:347:ALA:HB1	1.35	0.92
1:A:306:MET:HE1	1:A:351:HIS:CD2	2.05	0.91
1:A:310:TYR:CE1	1:A:347:ALA:HB1	2.06	0.90
2:H:35:ASP:OD1	2:H:99:GLU:OE2	1.90	0.90
1:A:238:TYR:CE2	1:A:281:PRO:HA	2.07	0.90
1:A:226:TYR:CB	1:A:358:LEU:HD22	2.00	0.89
1:A:226:TYR:HB2	1:A:358:LEU:HD22	1.55	0.89
1:A:238:TYR:CE2	1:A:281:PRO:CA	2.59	0.86
1:A:299:GLN:HE22	1:A:357:ASN:CB	1.84	0.85
1:A:306:MET:HE2	1:A:351:HIS:HB2	1.59	0.85
1:A:223:TRP:HZ2	1:A:300:MET:HE1	1.42	0.84
1:A:272:LEU:HD23	1:A:276:LEU:CD1	2.07	0.84
1:A:238:TYR:CD2	1:A:281:PRO:HB3	2.12	0.84
2:H:16:ALA:O	2:H:86:LEU:HG	1.79	0.82
1:A:310:TYR:CE1	1:A:347:ALA:HB3	2.13	0.82
1:A:299:GLN:NE2	1:A:357:ASN:CB	2.40	0.81
1:A:356:SER:O	1:A:359:GLN:CG	2.30	0.80
3:L:36:TYR:HE2	3:L:89:GLN:HG2	1.46	0.80
2:H:67:LYS:HZ1	2:H:90:ASP:CG	1.90	0.80
3:L:23:CYS:HG	3:L:88:CYS:HG	1.16	0.79
1:A:165:ALA:O	1:A:169:GLU:OE2	2.01	0.79
1:A:137:ASN:HD21	1:A:335:GLN:NE2	1.81	0.78
1:A:223:TRP:CZ2	1:A:300:MET:HE1	2.19	0.77
1:A:229:TYR:HB3	1:A:362:ARG:HD2	1.67	0.76
1:A:255:TRP:CG	1:A:260:THR:HG1	2.04	0.74
1:A:188:TRP:O	1:A:192:THR:HG23	1.88	0.73
1:A:230:CYS:SG	1:A:366:GLU:O	2.46	0.73
1:A:262:LYS:HB2	1:A:264:ARG:HG2	1.69	0.73
1:A:302:TRP:O	1:A:305:LEU:HG	1.89	0.72
1:A:134:GLU:O	1:A:138:ILE:HG12	1.90	0.71
1:A:299:GLN:CB	1:A:302:TRP:HD1	2.00	0.71
1:A:141:HIS:CD2	1:A:341:HIS:HD1	2.09	0.70
1:A:282:THR:OG1	1:A:300:MET:HE2	1.90	0.69
1:A:161:MET:HG2	1:A:167:LEU:HD22	1.74	0.69
1:A:301:GLY:O	1:A:304:PHE:HB3	1.93	0.69
1:A:272:LEU:HD23	1:A:276:LEU:HG	1.76	0.67
3:L:39:LYS:HE2	3:L:81:GLU:O	1.94	0.67
1:A:161:MET:O	1:A:167:LEU:HD21	1.94	0.67
1:A:226:TYR:HB3	1:A:358:LEU:HD22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD23	1:A:276:LEU:CG	2.24	0.66
1:A:282:THR:CB	1:A:300:MET:HE2	2.25	0.66
1:A:265:GLN:HG2	1:A:265:GLN:O	1.96	0.66
1:A:260:THR:HB	1:A:261:PRO:HA	1.78	0.65
1:A:226:TYR:HB3	1:A:358:LEU:CD2	2.26	0.65
2:H:67:LYS:NZ	2:H:90:ASP:CG	2.54	0.65
3:L:2:ILE:HD13	3:L:29:ILE:HG22	1.79	0.65
1:A:297:VAL:CG1	1:A:361:PHE:HD2	2.09	0.65
1:A:137:ASN:ND2	1:A:335:GLN:NE2	2.46	0.64
1:A:161:MET:HE2	1:A:167:LEU:HD13	1.79	0.64
1:A:187:SER:OG	1:A:341:HIS:HE1	1.79	0.64
1:A:248:SER:OG	1:A:270:VAL:HG21	1.98	0.64
1:A:272:LEU:O	1:A:276:LEU:HG	1.98	0.64
1:A:321:ILE:HG23	1:A:325:PHE:CE2	2.33	0.64
1:A:323:GLU:OE2	1:A:336:SER:N	2.30	0.64
1:A:306:MET:HE2	1:A:351:HIS:CB	2.27	0.63
3:L:61:ARG:HB2	3:L:76:ASN:O	1.98	0.63
1:A:152:GLY:O	1:A:156:MET:HB2	1.99	0.63
1:A:334:PHE:N	1:A:338:GLN:OE1	2.32	0.63
1:A:238:TYR:CE2	1:A:281:PRO:HB3	2.35	0.62
1:A:243:CYS:O	1:A:247:ILE:HD13	1.99	0.62
1:A:238:TYR:CE2	1:A:281:PRO:CB	2.83	0.62
1:A:352:PHE:HA	1:A:355:VAL:HG12	1.82	0.61
1:A:172:VAL:HG12	1:A:222:PRO:HA	1.81	0.61
1:A:248:SER:OG	1:A:270:VAL:CG2	2.49	0.61
1:A:238:TYR:HD2	1:A:281:PRO:HB3	1.64	0.61
1:A:312:THR:O	1:A:316:LEU:HB2	2.01	0.61
1:A:260:THR:HA	1:A:262:LYS:HG2	1.81	0.60
1:A:238:TYR:HE2	1:A:281:PRO:HA	1.43	0.60
1:A:286:THR:HG23	1:A:291:PHE:HA	1.83	0.60
1:A:314:ALA:O	1:A:317:TYR:HD1	1.85	0.59
3:L:2:ILE:HD12	3:L:93:SER:HB3	1.83	0.59
1:A:337:HIS:CD2	1:A:341:HIS:CD2	2.90	0.59
1:A:252:VAL:CG1	1:A:267:ARG:HA	2.25	0.59
1:A:248:SER:O	1:A:252:VAL:HG23	2.03	0.59
1:A:137:ASN:HD21	1:A:335:GLN:HE21	1.48	0.58
1:A:277:SER:O	1:A:281:PRO:CD	2.51	0.58
1:A:147:LEU:O	1:A:151:LEU:HD13	2.02	0.58
1:A:306:MET:CE	1:A:351:HIS:HB2	2.34	0.58
2:H:67:LYS:NZ	2:H:90:ASP:OD1	2.36	0.58
2:H:6:GLN:HA	2:H:21:THR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:HG21	2:H:86:LEU:CD1	2.34	0.57
1:A:238:TYR:HE2	1:A:281:PRO:N	2.02	0.57
1:A:320:ARG:O	1:A:323:GLU:OE1	2.22	0.56
1:A:278:GLY:O	1:A:281:PRO:HG2	2.05	0.56
1:A:361:PHE:O	1:A:365:LEU:HD13	2.06	0.56
1:A:172:VAL:HG13	1:A:222:PRO:HA	1.84	0.55
1:A:249:ALA:N	1:A:270:VAL:HG11	2.21	0.55
1:A:361:PHE:O	1:A:365:LEU:CD1	2.55	0.55
3:L:32:PHE:HB2	3:L:92:TRP:HB2	1.88	0.55
1:A:295:THR:HG23	1:A:301:GLY:HA3	1.88	0.55
1:A:338:GLN:O	1:A:342:VAL:HG23	2.07	0.55
1:A:297:VAL:HG12	1:A:361:PHE:HD2	1.72	0.54
1:A:138:ILE:HD12	1:A:192:THR:HG22	1.89	0.54
1:A:187:SER:OG	1:A:341:HIS:CE1	2.58	0.54
2:H:104:TRP:CZ3	2:H:106:ALA:HB2	2.42	0.53
1:A:359:GLN:HG3	1:A:360:GLU:N	2.23	0.53
2:H:61:ASN:HB3	2:H:64:PHE:HD2	1.73	0.53
1:A:297:VAL:HG11	1:A:361:PHE:HD2	1.72	0.53
2:H:29:PHE:CE2	2:H:72:VAL:HG21	2.44	0.52
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.91	0.52
1:A:299:GLN:O	1:A:303:PHE:N	2.37	0.52
3:L:36:TYR:CE2	3:L:89:GLN:HG2	2.37	0.52
1:A:352:PHE:O	1:A:355:VAL:HG12	2.10	0.52
1:A:365:LEU:HD13	1:A:365:LEU:H	1.74	0.51
2:H:6:GLN:H	2:H:110:GLN:HE22	1.59	0.51
3:L:83:PHE:HB3	3:L:106:ILE:HD13	1.92	0.51
1:A:335:GLN:HG2	1:A:338:GLN:HG2	1.93	0.51
1:A:277:SER:O	1:A:281:PRO:HD2	2.11	0.51
1:A:199:LYS:HG3	1:A:200:VAL:N	2.26	0.50
1:A:302:TRP:HZ2	1:A:353:TYR:CD2	2.29	0.50
1:A:249:ALA:HA	6:A:506:HOH:O	2.11	0.50
1:A:305:LEU:HD13	1:A:350:VAL:HG11	1.94	0.50
1:A:234:PRO:O	1:A:237:ILE:HG12	2.12	0.49
3:L:10:SER:HB2	3:L:103:LYS:HE2	1.93	0.49
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.47	0.49
1:A:187:SER:O	1:A:191:HIS:HD2	1.96	0.49
2:H:70:PHE:CE1	2:H:81:MET:HG3	2.48	0.49
1:A:282:THR:HB	1:A:300:MET:CE	2.42	0.49
1:A:118:MET:O	1:A:196:HIS:HA	2.13	0.49
2:H:67:LYS:NZ	2:H:90:ASP:OD2	2.46	0.49
1:A:137:ASN:OD1	1:A:337:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HG13	1:A:238:TYR:HD1	1.78	0.48
2:H:103:ALA:HB3	3:L:91:PHE:HB2	1.95	0.48
1:A:298:GLY:C	1:A:299:GLN:HG3	2.39	0.48
1:A:365:LEU:O	1:A:365:LEU:HD22	2.13	0.48
1:A:249:ALA:HA	1:A:270:VAL:HG11	1.95	0.48
1:A:297:VAL:HG12	1:A:361:PHE:CD2	2.48	0.48
1:A:169:GLU:OE1	1:A:226:TYR:CE1	2.67	0.48
1:A:220:PHE:HD2	1:A:242:VAL:HG11	1.78	0.47
2:H:62:GLN:OE1	2:H:65:LYS:HE3	2.14	0.47
1:A:249:ALA:CA	1:A:270:VAL:HG11	2.45	0.47
3:L:91:PHE:HA	3:L:96:TYR:CD1	2.50	0.47
1:A:265:GLN:O	1:A:268:ALA:HB3	2.15	0.47
2:H:6:GLN:H	2:H:110:GLN:NE2	2.13	0.47
1:A:321:ILE:HG23	1:A:325:PHE:CD2	2.49	0.47
1:A:116:PRO:O	1:A:118:MET:HE2	2.16	0.46
1:A:306:MET:CE	1:A:351:HIS:CB	2.91	0.46
2:H:89:GLU:N	2:H:89:GLU:OE1	2.48	0.46
3:L:39:LYS:CE	3:L:81:GLU:O	2.64	0.46
1:A:180:ALA:HA	1:A:215:LEU:HD13	1.97	0.46
3:L:4:MET:HE1	3:L:33:LEU:HD12	1.97	0.46
1:A:169:GLU:OE1	1:A:226:TYR:OH	2.31	0.46
1:A:340:PHE:O	1:A:344:VAL:HG23	2.16	0.46
2:H:73:ASP:CG	2:H:76:SER:OG	2.60	0.45
1:A:300:MET:HA	1:A:303:PHE:HB3	1.98	0.45
3:L:30:HIS:ND1	3:L:92:TRP:CE2	2.85	0.45
1:A:226:TYR:CB	1:A:358:LEU:CD2	2.78	0.45
1:A:141:HIS:CD2	1:A:341:HIS:ND1	2.79	0.45
1:A:335:GLN:HG2	1:A:338:GLN:CD	2.42	0.45
1:A:161:MET:CG	1:A:167:LEU:HD22	2.46	0.45
3:L:2:ILE:CD1	3:L:93:SER:HB3	2.45	0.45
1:A:362:ARG:HA	1:A:362:ARG:HD3	1.75	0.45
1:A:302:TRP:HZ2	1:A:353:TYR:HD2	1.65	0.44
1:A:297:VAL:CG1	1:A:361:PHE:CD2	2.96	0.44
2:H:29:PHE:CZ	2:H:72:VAL:CG2	3.00	0.44
2:H:12:VAL:HG21	2:H:86:LEU:HD12	1.99	0.44
1:A:338:GLN:HE21	1:A:338:GLN:HB3	1.56	0.43
2:H:67:LYS:CE	2:H:90:ASP:OD2	2.67	0.43
1:A:156:MET:HA	1:A:170:LYS:HZ2	1.83	0.43
3:L:89:GLN:HB3	3:L:98:PHE:CD2	2.54	0.43
1:A:226:TYR:HA	1:A:229:TYR:HB2	2.01	0.42
1:A:262:LYS:CB	1:A:264:ARG:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:OE1	1:A:226:TYR:CZ	2.72	0.42
1:A:213:ALA:O	1:A:217:MET:HG3	2.20	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.86	0.41
1:A:236:LEU:C	1:A:236:LEU:HD23	2.44	0.41
2:H:29:PHE:HE2	2:H:72:VAL:HG21	1.84	0.41
1:A:317:TYR:CD1	1:A:318:ALA:N	2.88	0.41
1:A:161:MET:O	1:A:167:LEU:CD2	2.65	0.41
2:H:30:THR:HA	2:H:53:PRO:HB2	2.02	0.41
1:A:302:TRP:CZ2	1:A:353:TYR:CE2	3.08	0.41
1:A:238:TYR:CD2	1:A:281:PRO:CB	2.93	0.41
2:H:70:PHE:HE1	2:H:81:MET:HG3	1.84	0.41
2:H:97:ALA:HB1	2:H:105:PHE:HB3	2.03	0.41
1:A:137:ASN:ND2	1:A:335:GLN:HE22	2.15	0.41
1:A:141:HIS:CG	1:A:341:HIS:HD1	2.36	0.41
1:A:279:VAL:HA	1:A:282:THR:CG2	2.50	0.41
1:A:158:ARG:HG2	1:A:164:MET:HE3	2.03	0.40
1:A:280:VAL:N	1:A:281:PRO:HD2	2.35	0.40
1:A:303:PHE:C	1:A:305:LEU:HD12	2.46	0.40
3:L:37:GLN:HG3	3:L:86:TYR:CZ	2.55	0.40
2:H:29:PHE:CE2	2:H:72:VAL:CG2	3.04	0.40
1:A:176:PHE:HB2	1:A:222:PRO:HG3	2.02	0.40
3:L:29:ILE:O	3:L:92:TRP:HB2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:GLU:OE2	2:H:88:PHE:O[7_554]	1.77	0.43
1:A:366:GLU:OE2	2:H:88:PHE:C[7_554]	2.19	0.01

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	280/305 (92%)	273 (98%)	7 (2%)	0	100	100
2	H	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
3	L	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
All	All	502/531 (94%)	491 (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	240/262 (92%)	228 (95%)	12 (5%)	22	40
2	H	99/99 (100%)	94 (95%)	5 (5%)	21	39
3	L	90/90 (100%)	88 (98%)	2 (2%)	45	65
All	All	429/451 (95%)	410 (96%)	19 (4%)	25	45

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	267	ARG
1	A	271	PHE
1	A	282	THR
1	A	302	TRP
1	A	305	LEU
1	A	316	LEU
1	A	317	TYR
1	A	324	ARG
1	A	332	ILE
1	A	338	GLN
1	A	365	LEU
2	H	43	LYS
2	H	93	VAL
2	H	99	GLU

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Mol	Chain	Res	Type
2	H	100	THR
2	H	115	THR
3	L	76	ASN
3	L	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	299	GLN
1	A	335	GLN
1	A	351	HIS
1	A	357	ASN
1	A	359	GLN
2	H	39	GLN
3	L	3	GLN
3	L	38	GLN
3	L	76	ASN
3	L	89	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	SO4	L	201	-	4,4,4	0.25	0	6,6,6	0.09	0
5	SO4	A	402	-	4,4,4	0.26	0	6,6,6	0.07	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, 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	280/305 (91%)	0.82	32 (11%) 10 9	44, 85, 127, 181	5 (1%)
2	H	119/119 (100%)	0.28	2 (1%) 69 66	44, 71, 89, 125	0
3	L	107/107 (100%)	-0.28	0 100 100	33, 44, 64, 90	0
All	All	506/531 (95%)	0.46	34 (6%) 24 23	33, 69, 117, 181	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	5.2
1	A	163	PHE	3.9
1	A	165	ALA	3.9
1	A	260	THR	3.5
1	A	162	TYR	3.5
1	A	258	PHE	3.4
1	A	271	PHE	3.3
1	A	161	MET	3.2
1	A	255	TRP	3.1
1	A	317	TYR	3.1
1	A	363	TYR	3.0
2	H	119	ALA	3.0
1	A	261	PRO	2.9
1	A	315	GLY	2.8
1	A	168	GLN	2.8
1	A	368	GLY	2.7
1	A	359	GLN	2.6
1	A	364	GLY	2.6
1	A	303	PHE	2.4
1	A	287	ILE	2.4
1	A	297	VAL	2.4
1	A	302	TRP	2.3
1	A	275	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	-1	GLY	2.2
1	A	274	LEU	2.2
1	A	340	PHE	2.2
1	A	289	GLU	2.2
1	A	228	PHE	2.1
1	A	259	ALA	2.1
1	A	164	MET	2.1
1	A	314	ALA	2.0
2	H	118	ALA	2.0
1	A	170	LYS	2.0
1	A	166	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
5	SO4	L	201	5/5	0.77	0.23	118,118,118,118	0
4	ZN	A	401	1/1	0.96	0.08	63,63,63,63	0
5	SO4	A	402	5/5	0.97	0.06	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.