



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:28 pm BST

PDB ID : 5LXG
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 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 : 2.11
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) : 2.11

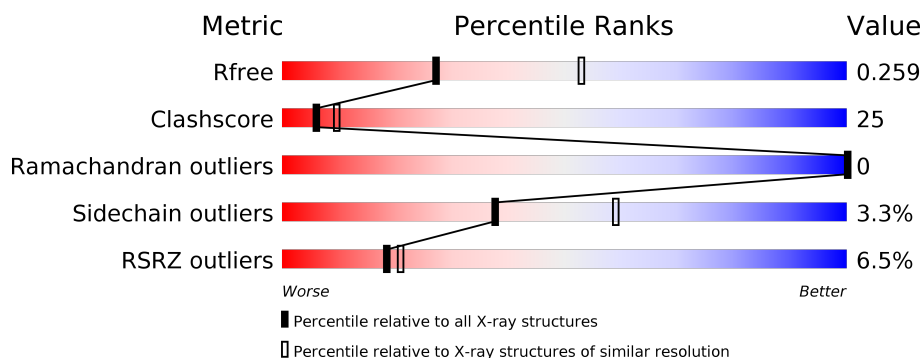
1 Overall quality at a glance

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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 on 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% 58% 32% 8%
2	H	119	 3% 70% 30%
3	L	107	 79% 20%

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

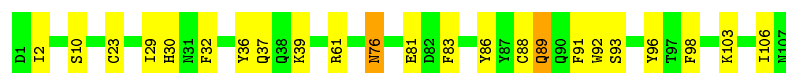


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- 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		

- Molecule 1: Adiponectin receptor protein 1



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 29.66 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.1 (26.66-2.73) 98.3 (29.66-2.73)	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 (5.01%)	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)	0.29 , 73.4	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/2368	0.64	0/3217
2	H	0.38	0/951	0.61	0/1291
3	L	0.31	0/840	0.53	0/1140
All	All	0.40	0/4159	0.61	0/5648

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	2286	0	2271	149	2
2	H	927	0	886	28	2
3	L	820	0	786	18	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	194	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 (194) 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:306:MET:HE1	1:A:351:HIS:CD2	1.98	0.99
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
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: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: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
1:A:306:MET:HE1	1:A:351:HIS:HD2	1.42	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:23:CYS:HG	3:L:88:CYS:HG	1.14	0.80
3:L:36:TYR:HE2	3:L:89:GLN:HG2	1.46	0.80
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:229:TYR:HB3	1:A:362:ARG:HD2	1.67	0.76
2:H:67:LYS:HZ1	2:H:90:ASP:CG	1.90	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:O	1:A:192:THR:HG23	1.88	0.73
1:A:262:LYS:HB2	1:A:264:ARG:HG2	1.69	0.73
1:A:230:CYS:SG	1:A:366:GLU:O	2.46	0.73
1:A:302:TRP:O	1:A:305:LEU:HG	1.89	0.72
1:A:282:THR:HB	1:A:300:MET:HE1	1.69	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: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
1:A:272:LEU:HD23	1:A:276:LEU:CG	2.24	0.66
1:A:265:GLN:O	1:A:265:GLN:HG2	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
3:L:2:ILE:HD13	3:L:29:ILE:HG22	1.79	0.65
1:A:306:MET:HE1	1:A:351:HIS:CG	2.31	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: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
3:L:61:ARG:HB2	3:L:76:ASN:O	1.98	0.63
1:A:282:THR:CB	1:A:300:MET:HE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG23	1:A:291:PHE:HA	1.83	0.60
2:H:67:LYS:NZ	2:H:90:ASP:CG	2.54	0.60
1:A:306:MET:HE1	1:A:351:HIS:CB	2.31	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
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
1:A:359:GLN:HG3	1:A:360:GLU:N	2.23	0.54
2:H:104:TRP:CZ3	2:H:106:ALA:HB2	2.42	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:38:LYS:HB2	2:H:48:ILE:HD11	1.91	0.52
2:H:29:PHE:CE2	2:H:72:VAL:HG21	2.44	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:H	1:A:365:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:O	1:A:281:PRO:HD2	2.11	0.51
1:A:223:TRP:HZ2	1:A:300:MET:CE	2.24	0.50
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: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:237:ILE:HG13	1:A:238:TYR:HD1	1.78	0.48
1:A:137:ASN:OD1	1:A:337:HIS:HD2	1.96	0.48
2:H:103:ALA:HB3	3:L:91:PHE:HB2	1.95	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
3:L:91:PHE:HA	3:L:96:TYR:CD1	2.50	0.47
1:A:249:ALA:CA	1:A:270:VAL:HG11	2.45	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:306:MET:HE1	1:A:351:HIS:HB2	1.95	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
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
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: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:282:THR:HB	1:A:300:MET:CE	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:169:GLU:OE1	1:A:226:TYR:CZ	2.72	0.42
1:A:223:TRP:HZ2	1:A:300:MET:HE1	1.83	0.42
1:A:298:GLY:C	1:A:299:GLN:HG3	2.39	0.42
1:A:306:MET:HE2	1:A:351:HIS:HB2	2.01	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
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
2:H:73:ASP:CG	2:H:76:SER:OG	2.60	0.41
1:A:280:VAL:N	1:A:281:PRO:HD2	2.35	0.40
3:L:37:GLN:HG3	3:L:86:TYR:CZ	2.55	0.40
1:A:335:GLN:HG2	1:A:338:GLN:CD	2.42	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%)	231 (96%)	9 (4%)	33	54
2	H	99/99 (100%)	96 (97%)	3 (3%)	41	61
3	L	90/90 (100%)	88 (98%)	2 (2%)	52	71
All	All	429/451 (95%)	415 (97%)	14 (3%)	38	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	PHE
1	A	282	THR
1	A	302	TRP
1	A	305	LEU
1	A	317	TYR

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Mol	Chain	Res	Type
1	A	324	ARG
1	A	338	GLN
1	A	359	GLN
1	A	365	LEU
2	H	93	VAL
2	H	100	THR
2	H	115	THR
3	L	76	ASN
3	L	89	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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
3	L	3	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 carbohydrates 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	0.15	0	6,6,6	0.06	0
5	SO4	A	402	-	4,4,4	0.15	0	6,6,6	0.04	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%)	0.50	29 (10%) 6 6	48, 86, 131, 186	5 (1%)
2	H	119/119 (100%)	0.07	4 (3%) 45 50	44, 71, 89, 125	0
3	L	107/107 (100%)	-0.30	0 100 100	33, 44, 64, 90	0
All	All	506/531 (95%)	0.23	33 (6%) 18 21	33, 70, 118, 186	5 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	PHE	5.0
1	A	260	THR	4.9
1	A	268	ALA	4.7
1	A	261	PRO	4.7
1	A	262	LYS	4.3
1	A	255	TRP	4.2
2	H	119	ALA	4.2
1	A	259	ALA	3.6
1	A	264	ARG	3.5
1	A	109	TYR	3.4
1	A	265	GLN	3.1
1	A	363	TYR	3.1
1	A	263	HIS	3.1
2	H	118	ALA	3.0
1	A	256	ASP	3.0
1	A	165	ALA	3.0
2	H	116	VAL	2.9
1	A	302	TRP	2.8
1	A	167	LEU	2.6
1	A	325	PHE	2.6
1	A	-1	GLY	2.6
2	H	86	LEU	2.5
1	A	257	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	361	PHE	2.4
1	A	254	GLN	2.4
1	A	328	GLY	2.3
1	A	272	LEU	2.3
1	A	296	THR	2.3
1	A	292	VAL	2.2
1	A	334	PHE	2.1
1	A	327	PRO	2.1
1	A	170	LYS	2.0
1	A	301	GLY	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 carbohydrates 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	0.87	0.29	118,118,118,118	0
4	ZN	A	401	1/1	0.96	0.21	63,63,63,63	0
5	SO4	A	402	5/5	0.98	0.07	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.