



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 PM UTC

PDB ID : 4ERS / pdb_00004ers
Title : A Molecular Basis for Negative Regulation of the Glucagon Receptor
Authors : Murray, J.M.; Koth, C.M.; Mukund, S.
Deposited on : 2012-04-20
Resolution : 2.64 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

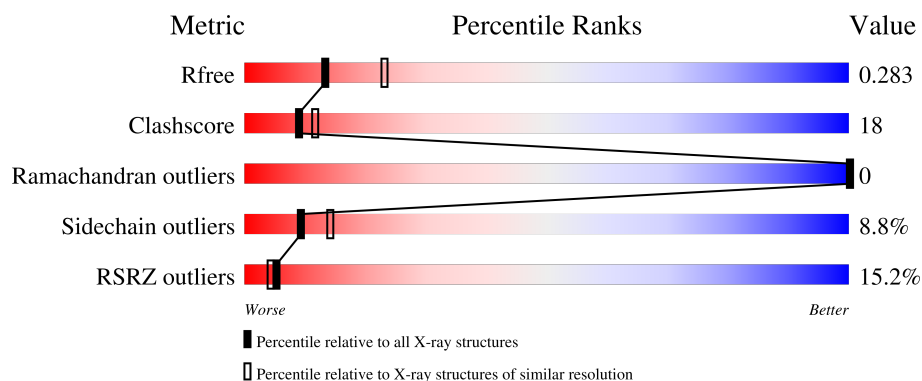
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	L	214	14% 64% 32% .
2	H	231	15% 66% 29% .
3	A	96	18% 60% 34% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4285 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 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1633	1015	280	332	6			

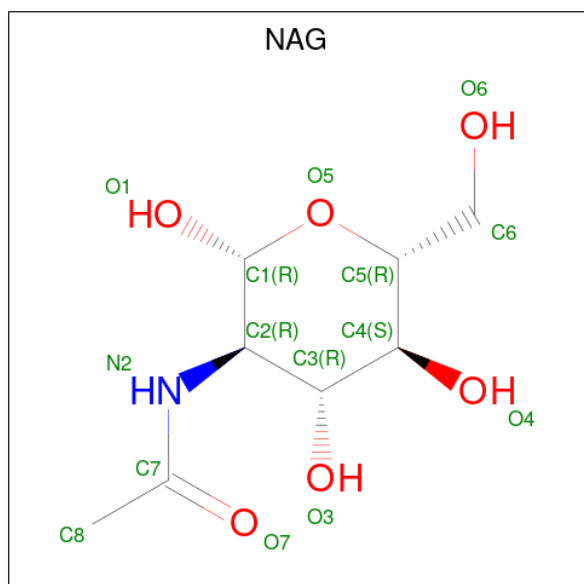
- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	231	Total	C	N	O	S	0	0	0
			1756	1107	297	344	8			

- Molecule 3 is a protein called Glucagon receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	96	Total	C	N	O	S	0	0	0
			792	508	143	134	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

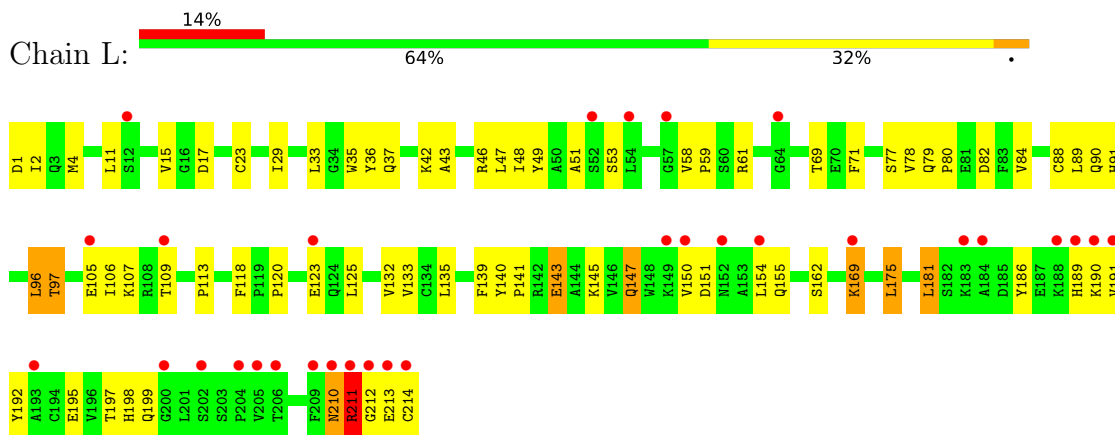
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	27	Total	O	0	0
			27	27		
5	H	38	Total	O	0	0
			38	38		
5	A	11	Total	O	0	0
			11	11		

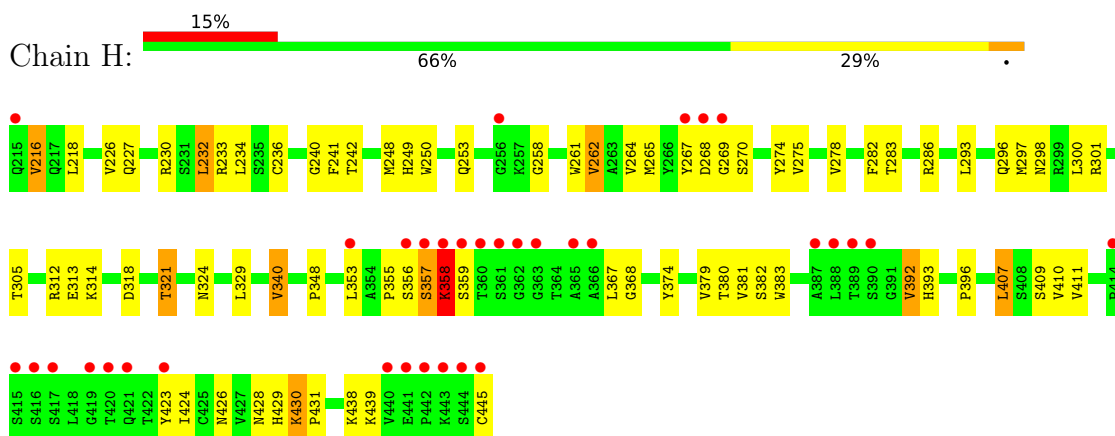
3 Residue-property plots [i](#)

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.

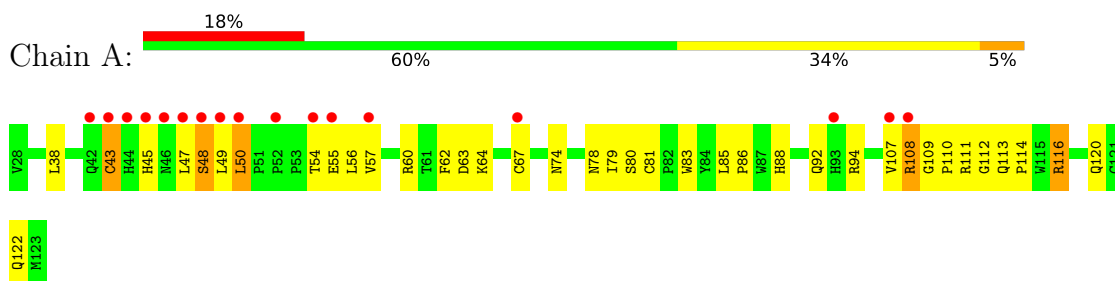
- Molecule 1: Fab light chain



- Molecule 2: Fab heavy chain



- Molecule 3: Glucagon receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.41Å 62.25Å 104.94Å 90.00° 93.91° 90.00°	Depositor
Resolution (Å)	43.46 – 2.64 43.46 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.46-2.64) 98.5 (43.46-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.231 , 0.279 0.246 , 0.283	Depositor DCC
R_{free} test set	895 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.3	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	0.88	EDS
Total number of atoms	4285	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: 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	L	0.38	0/1666	0.79	2/2259 (0.1%)
2	H	0.43	0/1799	0.90	8/2448 (0.3%)
3	A	0.58	1/826 (0.1%)	0.95	3/1132 (0.3%)
All	All	0.44	1/4291 (0.0%)	0.87	13/5839 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	110	PRO	N-CD	5.35	1.55	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	268	ASP	N-CA-C	14.77	126.88	111.07
1	L	169	LYS	N-CA-C	10.57	122.56	111.14
2	H	269	GLY	N-CA-C	-7.89	90.42	113.30
2	H	321	THR	N-CA-C	5.98	117.87	111.36
3	A	109	GLY	CA-C-N	-5.73	112.69	119.05
3	A	109	GLY	C-N-CA	-5.73	112.69	119.05
2	H	270	SER	N-CA-C	-5.56	105.27	113.61
3	A	107	VAL	N-CA-C	5.45	116.08	108.89
2	H	357	SER	CB-CA-C	-5.44	110.28	116.54
1	L	211	ARG	N-CA-C	5.18	118.89	112.47
2	H	267	TYR	CA-C-N	5.16	127.14	120.44
2	H	267	TYR	C-N-CA	5.16	127.14	120.44
2	H	358	LYS	N-CA-C	5.03	116.84	111.36

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	L	1633	0	1590	53	0
2	H	1756	0	1704	59	0
3	A	792	0	716	45	0
4	A	28	0	26	3	0
5	A	11	0	0	1	0
5	H	38	0	0	2	0
5	L	27	0	0	3	0
All	All	4285	0	4036	151	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 18.

All (151) 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)
3:A:74:ASN:HD21	4:A:202:NAG:C1	0.94	1.58
3:A:47:LEU:HB3	3:A:60:ARG:HD3	1.22	1.13
3:A:45:HIS:O	3:A:48:SER:HB2	1.66	0.94
3:A:45:HIS:O	3:A:48:SER:CB	2.21	0.88
3:A:47:LEU:HD11	3:A:67:CYS:SG	2.13	0.88
3:A:47:LEU:HA	3:A:50:LEU:HD11	1.59	0.84
3:A:47:LEU:HA	3:A:50:LEU:CD1	2.08	0.83
3:A:63:ASP:O	3:A:64:LYS:HB2	1.80	0.82
3:A:74:ASN:HD21	4:A:202:NAG:C2	1.93	0.81
1:L:213:GLU:HB2	2:H:445:CYS:HB2	1.62	0.81
1:L:4:MET:HG2	1:L:97:THR:HG22	1.65	0.77
1:L:145:LYS:HB2	1:L:197:THR:HB	1.65	0.77
1:L:135:LEU:HD22	2:H:410:VAL:HG11	1.66	0.76
3:A:47:LEU:O	3:A:60:ARG:NH1	2.21	0.74
3:A:49:LEU:HD12	3:A:50:LEU:N	2.05	0.70
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.74	0.69
3:A:47:LEU:CD1	3:A:67:CYS:SG	2.80	0.69
3:A:45:HIS:O	3:A:48:SER:N	2.26	0.69
1:L:97:THR:HG23	5:L:316:HOH:O	1.92	0.68
2:H:348:PRO:HB3	2:H:374:TYR:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:50:LEU:O	3:A:60:ARG:NH2	2.27	0.67
2:H:430:LYS:NZ	2:H:430:LYS:HB3	2.10	0.66
2:H:232:LEU:HD13	2:H:233:ARG:N	2.10	0.66
2:H:248:MET:HB3	2:H:293:LEU:HD22	1.77	0.66
3:A:94:ARG:HB3	3:A:120:GLN:HB3	1.77	0.66
3:A:63:ASP:HB2	3:A:114:PRO:HB3	1.78	0.66
3:A:74:ASN:ND2	4:A:202:NAG:C2	2.57	0.66
1:L:150:VAL:HA	1:L:191:VAL:O	1.98	0.64
1:L:46:ARG:HD3	1:L:49:TYR:HB3	1.78	0.64
1:L:36:TYR:HE2	1:L:89:LEU:HB3	1.61	0.63
1:L:97:THR:CG2	5:L:316:HOH:O	2.46	0.63
3:A:56:LEU:HD12	5:A:303:HOH:O	1.99	0.62
1:L:4:MET:CG	1:L:97:THR:HG22	2.30	0.62
2:H:355:PRO:O	2:H:356:SER:HB3	2.01	0.61
3:A:47:LEU:HD13	3:A:60:ARG:HB2	1.81	0.61
3:A:47:LEU:HD22	3:A:50:LEU:HD11	1.83	0.60
1:L:150:VAL:HG12	1:L:155:GLN:NE2	2.17	0.59
1:L:120:PRO:HB2	1:L:125:LEU:HD21	1.84	0.59
3:A:45:HIS:HA	3:A:48:SER:HB2	1.83	0.59
3:A:45:HIS:C	3:A:48:SER:HB2	2.28	0.58
3:A:47:LEU:HB3	3:A:60:ARG:CD	2.15	0.58
1:L:175:LEU:HD12	1:L:175:LEU:C	2.28	0.58
2:H:226:VAL:O	2:H:340:VAL:HA	2.03	0.57
2:H:356:SER:O	2:H:357:SER:C	2.47	0.57
2:H:265:MET:HE2	2:H:286:ARG:CD	2.35	0.57
2:H:407:LEU:C	2:H:407:LEU:HD12	2.30	0.57
2:H:232:LEU:HB3	2:H:297:MET:HE3	1.87	0.56
2:H:298:ASN:ND2	5:H:516:HOH:O	2.38	0.56
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.41	0.56
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.88	0.55
2:H:318:ASP:HB3	2:H:321:THR:OG1	2.07	0.55
2:H:232:LEU:HD13	2:H:233:ARG:H	1.70	0.55
2:H:382:SER:HB3	2:H:426:ASN:HB2	1.89	0.55
1:L:2:ILE:O	1:L:97:THR:HG21	2.06	0.55
3:A:43:CYS:O	3:A:47:LEU:HG	2.07	0.54
3:A:108:ARG:HB3	3:A:112:GLY:HA2	1.90	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.88	0.54
2:H:393:HIS:N	2:H:410:VAL:O	2.37	0.53
2:H:368:GLY:HA2	2:H:383:TRP:CZ2	2.43	0.53
1:L:23:CYS:HB2	1:L:35:TRP:CH2	2.45	0.52
1:L:147:GLN:OE1	1:L:154:LEU:HD11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:VAL:CG2	1:L:189:HIS:HB3	2.40	0.52
3:A:45:HIS:C	3:A:48:SER:H	2.18	0.52
3:A:47:LEU:CG	3:A:67:CYS:SG	2.98	0.52
2:H:305:THR:OG1	2:H:340:VAL:HG13	2.11	0.51
3:A:111:ARG:HB2	3:A:113:GLN:OE1	2.10	0.51
2:H:367:LEU:O	2:H:410:VAL:HG13	2.11	0.51
2:H:356:SER:OG	2:H:359:SER:O	2.29	0.50
3:A:63:ASP:OD2	3:A:116:ARG:NH1	2.45	0.50
1:L:4:MET:HG2	1:L:97:THR:CG2	2.38	0.50
1:L:96:LEU:HB2	2:H:261:TRP:CG	2.47	0.50
1:L:118:PHE:HB2	1:L:133:VAL:CG2	2.42	0.50
2:H:410:VAL:HG12	2:H:411:VAL:N	2.25	0.50
2:H:321:THR:HG21	5:H:530:HOH:O	2.12	0.50
1:L:150:VAL:HG22	1:L:189:HIS:HB3	1.93	0.50
1:L:210:ASN:N	1:L:210:ASN:OD1	2.44	0.50
1:L:151:ASP:OD1	1:L:190:LYS:HB3	2.12	0.50
3:A:47:LEU:HG	3:A:67:CYS:SG	2.51	0.49
3:A:83:TRP:HA	3:A:88:HIS:CG	2.47	0.49
1:L:29:ILE:HG21	1:L:90:GLN:HG3	1.95	0.49
2:H:424:ILE:HD11	2:H:439:LYS:HD2	1.94	0.49
1:L:48:ILE:HG21	1:L:51:ALA:O	2.12	0.49
1:L:17:ASP:O	1:L:77:SER:HA	2.11	0.49
3:A:43:CYS:SG	3:A:62:PHE:HB2	2.53	0.49
3:A:81:CYS:SG	3:A:94:ARG:HB2	2.53	0.49
3:A:88:HIS:O	3:A:92:GLN:HB3	2.13	0.49
2:H:424:ILE:HG13	2:H:439:LYS:HA	1.95	0.49
2:H:368:GLY:HA2	2:H:383:TRP:CH2	2.49	0.48
1:L:135:LEU:CD2	2:H:410:VAL:HG11	2.39	0.48
1:L:33:LEU:HD13	1:L:71:PHE:CD1	2.49	0.47
1:L:61:ARG:NE	1:L:82:ASP:OD2	2.42	0.47
1:L:91:HIS:HA	1:L:96:LEU:HD13	1.96	0.47
1:L:118:PHE:CD2	2:H:353:LEU:HB3	2.50	0.47
1:L:58:VAL:HG13	1:L:59:PRO:HD2	1.95	0.47
1:L:118:PHE:HB2	1:L:133:VAL:HG22	1.95	0.47
2:H:297:MET:HB3	2:H:300:LEU:HD21	1.97	0.47
2:H:216:VAL:HG23	2:H:241:PHE:CD1	2.50	0.47
2:H:250:TRP:O	2:H:262:VAL:HG13	2.14	0.47
2:H:301:ARG:O	2:H:340:VAL:HG11	2.15	0.46
1:L:212:GLY:C	1:L:214:CYS:N	2.71	0.46
3:A:55:GLU:O	3:A:57:VAL:HG13	2.16	0.46
3:A:45:HIS:CA	3:A:48:SER:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:249:HIS:NE2	2:H:313:GLU:OE1	2.43	0.46
3:A:45:HIS:O	3:A:48:SER:CA	2.63	0.46
1:L:113:PRO:CB	1:L:139:PHE:HB3	2.43	0.46
2:H:282:PHE:HA	2:H:296:GLN:O	2.15	0.45
2:H:410:VAL:CG1	2:H:411:VAL:N	2.79	0.45
2:H:261:TRP:HZ2	2:H:264:VAL:HG12	1.81	0.45
2:H:216:VAL:HG23	2:H:241:PHE:HD1	1.81	0.45
2:H:380:THR:OG1	2:H:428:ASN:HB3	2.16	0.45
3:A:67:CYS:O	3:A:79:ILE:CD1	2.64	0.45
2:H:253:GLN:HG3	2:H:258:GLY:O	2.17	0.45
2:H:367:LEU:HD12	2:H:367:LEU:C	2.42	0.45
1:L:162:SER:OG	2:H:396:PRO:HG2	2.17	0.45
3:A:47:LEU:HD23	3:A:47:LEU:N	2.32	0.44
3:A:63:ASP:O	3:A:64:LYS:CB	2.59	0.44
1:L:42:LYS:HD2	1:L:43:ALA:H	1.83	0.44
1:L:140:TYR:CG	1:L:141:PRO:HA	2.53	0.44
2:H:265:MET:HE2	2:H:286:ARG:HD3	1.98	0.44
1:L:49:TYR:O	1:L:53:SER:HB2	2.17	0.44
2:H:312:ARG:O	2:H:329:LEU:HA	2.18	0.44
1:L:169:LYS:HG2	5:L:310:HOH:O	2.18	0.43
2:H:236:CYS:HB3	2:H:293:LEU:HB3	1.99	0.43
1:L:79:GLN:HB3	1:L:80:PRO:HD2	2.00	0.43
2:H:423:TYR:C	2:H:424:ILE:HD12	2.43	0.43
2:H:283:THR:HB	2:H:296:GLN:HB2	2.00	0.43
2:H:216:VAL:HA	2:H:240:GLY:HA3	2.00	0.43
2:H:392:VAL:HA	2:H:411:VAL:HA	2.01	0.42
2:H:264:VAL:O	2:H:264:VAL:HG13	2.18	0.42
1:L:11:LEU:C	1:L:11:LEU:HD12	2.45	0.42
2:H:227:GLN:H	2:H:230:ARG:HH11	1.65	0.42
2:H:274:TYR:HB3	2:H:278:VAL:HG23	2.00	0.42
2:H:381:VAL:HG11	2:H:409:SER:CB	2.49	0.42
3:A:47:LEU:CD2	3:A:50:LEU:HD11	2.50	0.42
2:H:358:LYS:HA	2:H:358:LYS:HD2	1.48	0.41
2:H:430:LYS:HB3	2:H:430:LYS:HZ2	1.81	0.41
2:H:429:HIS:CE1	2:H:431:PRO:HB2	2.54	0.41
3:A:49:LEU:HD12	3:A:49:LEU:C	2.46	0.41
1:L:147:GLN:HB3	1:L:195:GLU:HB3	2.03	0.41
3:A:85:LEU:HA	3:A:86:PRO:HD3	1.90	0.41
1:L:190:LYS:O	1:L:211:ARG:HG2	2.20	0.41
2:H:379:VAL:HG23	2:H:407:LEU:HD21	2.02	0.41
1:L:181:LEU:HD13	1:L:186:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:TYR:HA	1:L:192:TYR:OH	2.20	0.41
2:H:329:LEU:N	2:H:329:LEU:HD12	2.36	0.41
3:A:49:LEU:HD12	3:A:50:LEU:CA	2.51	0.41
3:A:79:ILE:HG22	3:A:80:SER:O	2.20	0.41
1:L:42:LYS:CD	1:L:43:ALA:H	2.34	0.41
1:L:198:HIS:CG	1:L:199:GLN:N	2.88	0.40
2:H:275:VAL:O	2:H:278:VAL:HG22	2.21	0.40
1:L:143:GLU:CD	1:L:143:GLU:H	2.28	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	L	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
2	H	229/231 (99%)	210 (92%)	19 (8%)	0	100	100
3	A	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
All	All	535/541 (99%)	503 (94%)	32 (6%)	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	L	187/187 (100%)	169 (90%)	18 (10%)	8	12
2	H	196/196 (100%)	182 (93%)	14 (7%)	13	22
3	A	85/88 (97%)	76 (89%)	9 (11%)	6	9
All	All	468/471 (99%)	427 (91%)	41 (9%)	9	14

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	15	VAL
1	L	69	THR
1	L	78	VAL
1	L	84	VAL
1	L	96	LEU
1	L	97	THR
1	L	105	GLU
1	L	106	ILE
1	L	107	LYS
1	L	109	THR
1	L	123	GLU
1	L	143	GLU
1	L	147	GLN
1	L	175	LEU
1	L	181	LEU
1	L	210	ASN
1	L	211	ARG
2	H	216	VAL
2	H	218	LEU
2	H	232	LEU
2	H	234	LEU
2	H	242	THR
2	H	262	VAL
2	H	314	LYS
2	H	324	ASN
2	H	340	VAL
2	H	358	LYS
2	H	392	VAL
2	H	407	LEU
2	H	430	LYS
2	H	438	LYS
3	A	38	LEU
3	A	43	CYS

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Mol	Chain	Res	Type
3	A	48	SER
3	A	50	LEU
3	A	54	THR
3	A	78	ASN
3	A	108	ARG
3	A	116	ARG
3	A	122	GLN

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

Mol	Chain	Res	Type
2	H	291	ASN
3	A	74	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	201	3	14,14,15	0.98	1 (7%)	17,19,21	1.70	4 (23%)
4	NAG	A	202	3	14,14,15	0.86	0	17,19,21	1.63	3 (17%)

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
4	NAG	A	201	3	-	0/6/23/26	0/1/1/1
4	NAG	A	202	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	NAG	O5-C1	-2.67	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	202	NAG	C1-C2-N2	-5.14	102.33	110.43
4	A	201	NAG	O5-C1-C2	-3.13	106.44	111.29
4	A	201	NAG	C3-C4-C5	-2.96	104.86	110.23
4	A	201	NAG	O5-C5-C6	2.72	112.95	107.66
4	A	202	NAG	O3-C3-C4	-2.35	104.83	110.38
4	A	201	NAG	O7-C7-N2	2.17	125.82	121.98
4	A	202	NAG	O5-C5-C4	-2.04	105.87	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	NAG	C8-C7-N2-C2
4	A	202	NAG	O7-C7-N2-C2
4	A	202	NAG	O5-C5-C6-O6
4	A	202	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	NAG	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	L	214/214 (100%)	0.98	31 (14%) 6 5	15, 42, 83, 142	0
2	H	231/231 (100%)	0.74	34 (14%) 6 4	16, 32, 98, 163	0
3	A	96/96 (100%)	1.04	17 (17%) 4 3	18, 36, 79, 93	0
All	All	541/541 (100%)	0.89	82 (15%) 5 4	15, 37, 83, 163	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	362	GLY	6.2
2	H	267	TYR	5.9
2	H	420	THR	5.8
1	L	52	SER	5.5
3	A	49	LEU	5.1
2	H	268	ASP	4.9
2	H	419	GLY	4.8
3	A	107	VAL	4.8
1	L	212	GLY	4.7
1	L	12	SER	4.6
2	H	360	THR	4.4
1	L	188	LYS	4.4
3	A	55	GLU	4.2
3	A	45	HIS	4.2
2	H	363	GLY	4.1
1	L	214	CYS	4.1
2	H	444	SER	4.0
3	A	50	LEU	3.8
3	A	54	THR	3.7
2	H	445	CYS	3.7
3	A	48	SER	3.7
2	H	215	GLN	3.7
2	H	365	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	359	SER	3.5
1	L	190	LYS	3.5
3	A	44	HIS	3.4
1	L	210	ASN	3.2
3	A	42	GLN	3.2
1	L	150	VAL	3.2
1	L	193	ALA	3.1
2	H	389	THR	3.1
2	H	358	LYS	3.1
2	H	357	SER	3.1
2	H	353	LEU	3.0
1	L	184	ALA	3.0
2	H	366	ALA	3.0
3	A	46	ASN	3.0
1	L	211	ARG	3.0
2	H	390	SER	2.9
2	H	417	SER	2.9
2	H	442	PRO	2.9
3	A	47	LEU	2.9
1	L	206	THR	2.9
3	A	52	PRO	2.8
2	H	361	SER	2.8
1	L	209	PHE	2.8
2	H	443	LYS	2.7
2	H	421	GLN	2.7
1	L	123	GLU	2.6
1	L	205	VAL	2.6
3	A	43	CYS	2.6
2	H	423	TYR	2.6
1	L	169	LYS	2.6
1	L	64	GLY	2.5
2	H	415	SER	2.5
1	L	149	LYS	2.5
3	A	108	ARG	2.5
3	A	67	CYS	2.5
1	L	213	GLU	2.4
1	L	191	VAL	2.4
3	A	57	VAL	2.4
1	L	189	HIS	2.4
1	L	109	THR	2.3
3	A	93	HIS	2.3
1	L	105	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	441	GLU	2.3
2	H	440	VAL	2.3
1	L	204	PRO	2.3
2	H	387	ALA	2.2
2	H	356	SER	2.2
2	H	269	GLY	2.2
2	H	416	SER	2.2
2	H	414	PRO	2.2
1	L	54	LEU	2.2
1	L	200	GLY	2.2
2	H	388	LEU	2.2
1	L	202	SER	2.2
1	L	183	LYS	2.1
1	L	154	LEU	2.1
2	H	256	GLY	2.1
1	L	152	ASN	2.1
1	L	57	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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	NAG	A	202	14/15	0.69	0.21	20,20,20,20	0
4	NAG	A	201	14/15	0.80	0.15	32,45,68,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.