



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:55 AM UTC

PDB ID : 8SM1 / pdb_00008sm1
Title : CRYSTAL STRUCTURE OF HUMAN ANTIBODY 769A9 IN COMPLEX
WITH EPSTEIN-BARR VIRUS MAJOR GLYCOPROTEIN GP350
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Deposited on : 2023-04-25
Resolution : 3.29 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

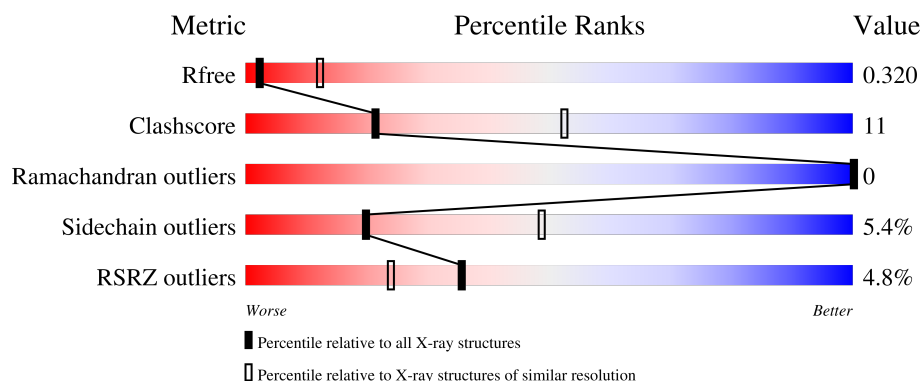
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	G	431	5% 75% 20% ..
2	H	228	7% 66% 22% 9%
3	L	215	2% 77% 20% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6513 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 Envelope glycoprotein gp350.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	420	Total	C	N	O	S	0	0	0
			3201	2024	519	641	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	426	HIS	-	expression tag	UNP P03200
G	427	HIS	-	expression tag	UNP P03200
G	428	HIS	-	expression tag	UNP P03200
G	429	HIS	-	expression tag	UNP P03200
G	430	HIS	-	expression tag	UNP P03200
G	431	HIS	-	expression tag	UNP P03200

- Molecule 2 is a protein called 769A9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1551	982	256	308	5			

- Molecule 3 is a protein called 769A9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1642	1030	277	331	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

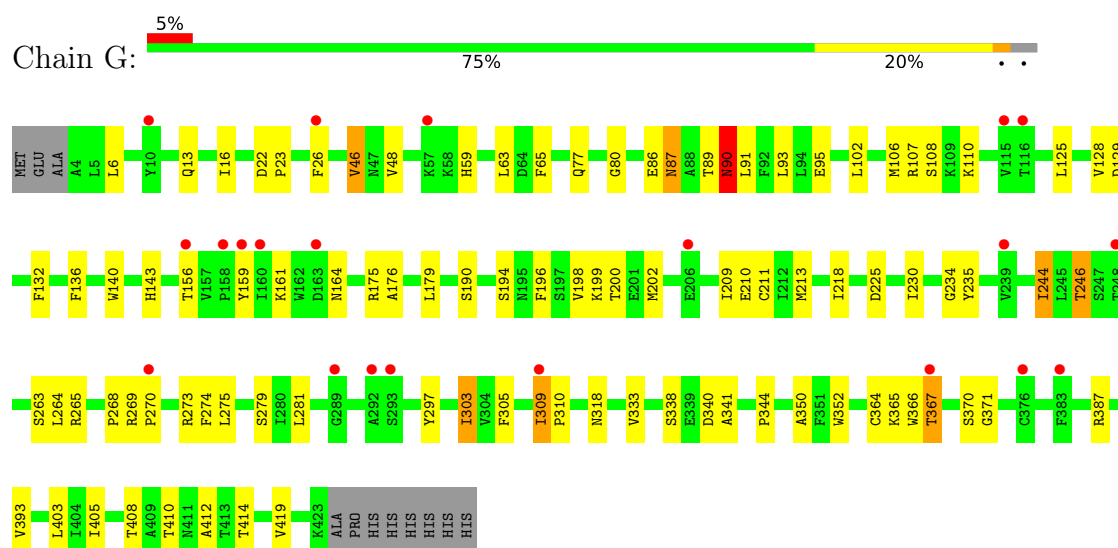
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	O	0	0
			1	1		

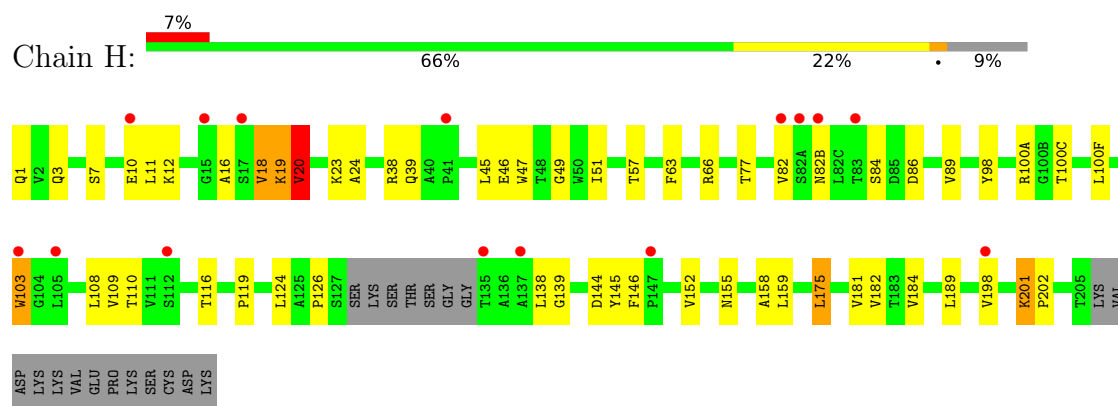
3 Residue-property plots

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.

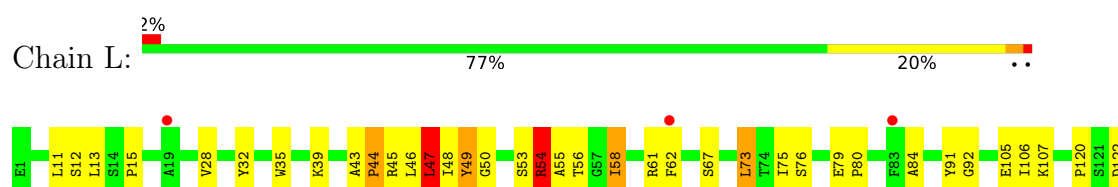
• Molecule 1: Envelope glycoprotein gp350

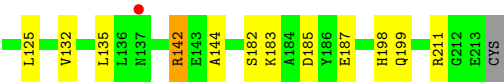


• Molecule 2: 769A9 Fab heavy chain



• Molecule 3: 769A9 Fab light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.08Å 54.68Å 137.22Å 90.00° 111.71° 90.00°	Depositor
Resolution (Å)	45.78 – 3.29 45.78 – 3.29	Depositor EDS
% Data completeness (in resolution range)	82.9 (45.78-3.29) 83.2 (45.78-3.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.258 , 0.298 0.279 , 0.320	Depositor DCC
R_{free} test set	733 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6513	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: GOL, 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	G	0.38	2/3278 (0.1%)	0.37	2/4486 (0.0%)
2	H	0.36	2/1591 (0.1%)	0.40	1/2177 (0.0%)
3	L	0.82	10/1678 (0.6%)	0.63	4/2278 (0.2%)
All	All	0.52	14/6547 (0.2%)	0.46	7/8941 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	20	VAL	C-O	-8.29	1.15	1.24
3	L	54	ARG	CA-C	-6.88	1.44	1.52
3	L	56	THR	CA-C	-6.41	1.44	1.52
1	G	80	GLY	C-O	-6.29	1.17	1.24
3	L	53	SER	CA-C	-6.03	1.45	1.52
1	G	86	GLU	CA-C	-5.71	1.45	1.52
3	L	56	THR	C-O	-5.55	1.17	1.23
3	L	53	SER	C-O	-5.54	1.17	1.23
2	H	20	VAL	CA-CB	-5.44	1.47	1.54
3	L	47	LEU	C-O	-5.36	1.16	1.23
3	L	45	ARG	C-O	-5.32	1.17	1.23
3	L	76	SER	CA-C	-5.22	1.46	1.53
3	L	47	LEU	CA-C	-5.16	1.47	1.52
3	L	44	PRO	CA-C	-5.03	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	49	TYR	N-CA-C	8.11	123.86	113.88
1	G	90	ASN	N-CA-C	-6.86	103.33	113.61
3	L	50	GLY	CA-C-N	6.38	133.73	121.54
3	L	50	GLY	C-N-CA	6.38	133.73	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	75	ILE	N-CA-C	-5.83	99.47	107.99
2	H	18	VAL	N-CA-CB	-5.39	101.84	111.92
1	G	86	GLU	N-CA-C	5.11	116.54	111.07

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	G	3201	0	3070	51	0
2	H	1551	0	1505	41	0
3	L	1642	0	1602	52	0
4	G	112	0	104	1	0
5	G	6	0	8	0	0
6	G	1	0	0	0	0
All	All	6513	0	6289	140	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 (140) 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:L:47:LEU:HD13	3:L:62:PHE:CD2	1.70	1.25
3:L:55:ALA:O	3:L:58:ILE:HG13	1.46	1.15
3:L:47:LEU:CD1	3:L:62:PHE:CE2	2.32	1.13
2:H:11:LEU:HD23	2:H:116:THR:HG22	1.22	1.11
3:L:47:LEU:HD11	3:L:62:PHE:HE2	1.08	1.06
3:L:47:LEU:CD1	3:L:62:PHE:CD2	2.41	1.03
3:L:47:LEU:HD11	3:L:62:PHE:CE2	1.89	1.03
3:L:47:LEU:O	3:L:58:ILE:HD12	1.57	1.03
3:L:47:LEU:HD13	3:L:62:PHE:HD2	1.16	0.99
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.36	0.90
2:H:11:LEU:CD2	2:H:116:THR:HG22	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ARG:HD2	2:H:82(B):ASN:CG	2.00	0.85
3:L:54:ARG:HD2	3:L:62:PHE:O	1.78	0.84
3:L:55:ALA:HB3	3:L:58:ILE:HD11	1.65	0.79
2:H:11:LEU:HD23	2:H:116:THR:CG2	2.11	0.77
3:L:61:ARG:HH22	3:L:79:GLU:CD	1.93	0.77
3:L:55:ALA:O	3:L:58:ILE:CG1	2.31	0.77
3:L:47:LEU:HD13	3:L:62:PHE:CE2	2.07	0.75
2:H:66:ARG:HD2	2:H:82(B):ASN:CB	2.18	0.74
3:L:15:PRO:HD3	3:L:107:LYS:HB3	1.68	0.73
3:L:47:LEU:O	3:L:58:ILE:CD1	2.35	0.73
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.71	0.71
3:L:61:ARG:NH2	3:L:79:GLU:CD	2.50	0.70
3:L:35:TRP:CE3	3:L:73:LEU:HD23	2.26	0.69
2:H:66:ARG:HD2	2:H:82(B):ASN:OD1	1.91	0.68
3:L:35:TRP:CE3	3:L:73:LEU:CD2	2.77	0.68
2:H:18:VAL:HG11	2:H:82:VAL:HG12	1.76	0.68
1:G:199:LYS:HD2	2:H:98:TYR:HB3	1.77	0.66
2:H:100(C):THR:HB	3:L:92:GLY:HA2	1.78	0.66
2:H:66:ARG:NH1	2:H:86:ASP:OD2	2.29	0.66
1:G:46:VAL:HG13	1:G:65:PHE:HB2	1.79	0.65
2:H:19:LYS:O	2:H:19:LYS:HD3	1.98	0.64
3:L:61:ARG:NH1	3:L:79:GLU:OE2	2.31	0.63
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.64	0.63
3:L:47:LEU:HA	3:L:58:ILE:HD13	1.81	0.62
1:G:246:THR:HG23	1:G:263:SER:HB3	1.80	0.62
3:L:183:LYS:NZ	3:L:187:GLU:OE2	2.33	0.61
1:G:341:ALA:O	1:G:387:ARG:NH1	2.33	0.61
3:L:61:ARG:HH22	3:L:79:GLU:CG	2.14	0.61
3:L:125:LEU:HB3	3:L:183:LYS:HE2	1.82	0.61
1:G:275:LEU:HB2	1:G:305:PHE:HZ	1.65	0.60
1:G:213:MET:HA	1:G:230:ILE:HA	1.82	0.60
3:L:61:ARG:NH2	3:L:79:GLU:OE2	2.34	0.60
2:H:38:ARG:HG3	2:H:46:GLU:HG3	1.82	0.59
2:H:184:VAL:HG21	2:H:189:LEU:HD21	1.83	0.59
2:H:63:PHE:O	2:H:66:ARG:HG3	2.03	0.59
1:G:297:TYR:HA	4:G:501:NAG:H61	1.85	0.58
3:L:47:LEU:CD1	3:L:62:PHE:HE2	1.78	0.58
1:G:87:ASN:O	1:G:90:ASN:OD1	2.21	0.57
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.86	0.57
1:G:309:ILE:HD12	1:G:310:PRO:HD2	1.86	0.57
3:L:61:ARG:HH22	3:L:79:GLU:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:ALA:HB3	2:H:82(B):ASN:H	1.71	0.55
3:L:47:LEU:CD1	3:L:62:PHE:HD2	1.95	0.55
1:G:196:PHE:HB3	1:G:218:ILE:HD12	1.89	0.55
3:L:35:TRP:CZ3	3:L:73:LEU:HD23	2.42	0.55
1:G:175:ARG:HB2	1:G:310:PRO:HG3	1.87	0.54
3:L:47:LEU:HA	3:L:58:ILE:CD1	2.36	0.54
1:G:16:ILE:HD11	1:G:235:TYR:HB3	1.89	0.54
1:G:367:THR:H	1:G:370:SER:HG	1.54	0.54
3:L:187:GLU:O	3:L:211:ARG:NH1	2.41	0.54
1:G:136:PHE:HB3	1:G:365:LYS:HD2	1.89	0.54
1:G:366:TRP:HD1	1:G:371:GLY:HA2	1.72	0.54
1:G:225:ASP:H	1:G:246:THR:HA	1.72	0.54
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.91	0.53
2:H:23:LYS:HA	2:H:77:THR:HG22	1.91	0.53
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.90	0.53
2:H:155:ASN:HB3	2:H:158:ALA:HB3	1.92	0.52
2:H:18:VAL:O	2:H:18:VAL:HG13	2.09	0.52
1:G:132:PHE:HB3	1:G:140:TRP:HB2	1.92	0.52
1:G:176:ALA:O	1:G:269:ARG:NH2	2.43	0.52
2:H:7:SER:O	2:H:20:VAL:HG13	2.11	0.51
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.93	0.51
1:G:279:SER:HB3	1:G:303:ILE:HG23	1.93	0.50
1:G:87:ASN:N	1:G:87:ASN:ND2	2.59	0.50
1:G:338:SER:HB2	1:G:412:ALA:HA	1.93	0.50
3:L:39:LYS:HG2	3:L:84:ALA:HB2	1.93	0.49
1:G:200:THR:HB	1:G:211:CYS:HB2	1.94	0.49
3:L:55:ALA:C	3:L:58:ILE:HG13	2.31	0.49
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.95	0.48
3:L:49:TYR:O	3:L:91:TYR:OH	2.29	0.48
3:L:142:ARG:O	3:L:142:ARG:HG3	2.11	0.48
2:H:1:GLN:OE1	2:H:1:GLN:N	2.47	0.48
3:L:61:ARG:NH2	3:L:79:GLU:HG2	2.29	0.48
1:G:344:PRO:HD2	1:G:410:THR:HG21	1.95	0.48
3:L:61:ARG:CZ	3:L:79:GLU:OE2	2.62	0.47
1:G:244:ILE:HG23	1:G:265:ARG:HB3	1.94	0.47
3:L:35:TRP:CD2	3:L:73:LEU:CD2	2.98	0.47
1:G:179:LEU:HB3	1:G:268:PRO:HG2	1.97	0.47
1:G:190:SER:O	1:G:194:SER:OG	2.26	0.47
1:G:403:LEU:HB3	1:G:419:VAL:HG23	1.96	0.47
2:H:181:VAL:HG21	3:L:135:LEU:HD22	1.96	0.47
1:G:77:GLN:HE21	1:G:90:ASN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:VAL:HB	1:G:63:LEU:HB2	1.96	0.47
3:L:182:SER:HB3	3:L:185:ASP:HB2	1.96	0.47
2:H:10:GLU:HB2	2:H:109:VAL:HG23	1.97	0.46
2:H:124:LEU:HB2	2:H:139:GLY:C	2.41	0.46
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.51	0.46
2:H:11:LEU:HD11	2:H:146:PHE:HE2	1.81	0.46
1:G:210:GLU:OE1	2:H:100(A):ARG:N	2.49	0.45
1:G:202:MET:HE2	1:G:209:ILE:HB	1.97	0.45
1:G:275:LEU:HB2	1:G:305:PHE:CZ	2.49	0.45
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.18	0.45
2:H:126:PRO:HB3	2:H:138:LEU:HB3	1.97	0.45
2:H:3:GLN:O	2:H:24:ALA:HA	2.17	0.45
1:G:129:ASP:OD1	1:G:143:HIS:ND1	2.46	0.45
3:L:12:SER:HA	3:L:105:GLU:HB2	1.97	0.45
2:H:89:VAL:HG22	2:H:108:LEU:HG	1.97	0.44
3:L:35:TRP:CD2	3:L:73:LEU:HD22	2.52	0.44
1:G:269:ARG:HB3	1:G:270:PRO:HD3	1.99	0.44
2:H:12:LYS:HD3	2:H:12:LYS:HA	1.66	0.44
1:G:22:ASP:OD2	1:G:108:SER:OG	2.35	0.44
1:G:95:GLU:OE1	1:G:273:ARG:HD2	2.18	0.43
2:H:100(F):LEU:HB2	2:H:103:TRP:CZ3	2.53	0.43
2:H:159:LEU:HD13	2:H:182:VAL:HG11	2.00	0.43
1:G:340:ASP:OD1	1:G:341:ALA:N	2.46	0.43
2:H:66:ARG:HD2	2:H:82(B):ASN:HB3	1.97	0.43
1:G:125:LEU:HD21	1:G:128:VAL:HG23	1.99	0.43
3:L:122:ASP:OD1	3:L:122:ASP:N	2.51	0.43
1:G:23:PRO:HD3	1:G:234:GLY:HA2	2.00	0.43
1:G:26:PHE:HD1	1:G:235:TYR:CZ	2.37	0.42
3:L:198:HIS:ND1	3:L:199:GLN:O	2.52	0.42
3:L:79:GLU:HB2	3:L:80:PRO:HD2	2.01	0.42
1:G:352:TRP:HH2	1:G:393:VAL:HG11	1.85	0.42
3:L:80:PRO:HA	3:L:106:ILE:HG13	2.02	0.42
1:G:333:VAL:HG21	1:G:405:ILE:HG21	2.01	0.41
3:L:32:TYR:HB3	3:L:91:TYR:O	2.20	0.41
2:H:66:ARG:NH1	2:H:86:ASP:CG	2.79	0.41
1:G:91:LEU:HA	1:G:107:ARG:HD3	2.02	0.41
1:G:107:ARG:HD2	1:G:274:PHE:CE1	2.55	0.41
3:L:11:LEU:HB3	3:L:13:LEU:HG	2.02	0.41
3:L:43:ALA:HB1	3:L:44:PRO:CD	2.51	0.41
3:L:61:ARG:H	3:L:61:ARG:HG2	1.63	0.41
1:G:408:THR:HB	1:G:414:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:ALA:HB1	1:G:403:LEU:HD11	2.02	0.40
1:G:13:GLN:HB3	1:G:143:HIS:HB3	2.03	0.40
1:G:198:VAL:HG21	1:G:264:LEU:HD21	2.03	0.40
1:G:213:MET:HB3	1:G:230:ILE:HG22	2.04	0.40
1:G:26:PHE:N	1:G:106:MET:O	2.55	0.40
1:G:93:LEU:HD23	1:G:273:ARG:HD3	2.03	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	G	418/431 (97%)	374 (90%)	44 (10%)	0	100	100
2	H	204/228 (90%)	191 (94%)	13 (6%)	0	100	100
3	L	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
All	All	834/874 (95%)	763 (92%)	71 (8%)	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	G	364/373 (98%)	344 (94%)	20 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	174/192 (91%)	164 (94%)	10 (6%)	18	47
3	L	184/185 (100%)	175 (95%)	9 (5%)	22	51
All	All	722/750 (96%)	683 (95%)	39 (5%)	20	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	6	LEU
1	G	46	VAL
1	G	59	HIS
1	G	87	ASN
1	G	89	THR
1	G	90	ASN
1	G	102	LEU
1	G	110	LYS
1	G	156	THR
1	G	159	TYR
1	G	161	LYS
1	G	164	ASN
1	G	244	ILE
1	G	246	THR
1	G	281	LEU
1	G	303	ILE
1	G	309	ILE
1	G	318	ASN
1	G	364	CYS
1	G	367	THR
2	H	19	LYS
2	H	20	VAL
2	H	84	SER
2	H	103	TRP
2	H	110	THR
2	H	144	ASP
2	H	152	VAL
2	H	175	LEU
2	H	198	VAL
2	H	201	LYS
3	L	28	VAL
3	L	46	LEU
3	L	47	LEU
3	L	48	ILE

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Mol	Chain	Res	Type
3	L	54	ARG
3	L	58	ILE
3	L	67	SER
3	L	73	LEU
3	L	142	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	9	GLN
1	G	67	GLN
1	G	77	GLN
1	G	87	ASN
1	G	121	GLN
2	H	3	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](#)

9 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	G	506	1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	G	505	1	14,14,15	0.25	0	17,19,21	0.44	0
5	GOL	G	509	-	5,5,5	0.22	0	5,5,5	0.52	0
4	NAG	G	507	1	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	G	503	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	G	508	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	G	504	1	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	G	502	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	G	501	1	14,14,15	0.18	0	17,19,21	0.43	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
4	NAG	G	506	1	-	3/6/23/26	0/1/1/1
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1
5	GOL	G	509	-	-	1/4/4/4	-
4	NAG	G	507	1	-	3/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	4/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	501	NAG	C4-C5-C6-O6
4	G	505	NAG	O5-C5-C6-O6
4	G	501	NAG	O5-C5-C6-O6
4	G	505	NAG	C4-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	G	502	NAG	C4-C5-C6-O6
4	G	502	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	502	NAG	O7-C7-N2-C2
4	G	504	NAG	C4-C5-C6-O6
4	G	506	NAG	O5-C5-C6-O6
4	G	507	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
4	G	506	NAG	C3-C2-N2-C7
4	G	507	NAG	C3-C2-N2-C7
5	G	509	GOL	O2-C2-C3-O3
4	G	506	NAG	C1-C2-N2-C7
4	G	507	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	501	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	420/431 (97%)	0.54	21 (5%) 34 23	41, 67, 105, 129	0
2	H	208/228 (91%)	0.76	15 (7%) 21 15	47, 79, 109, 120	0
3	L	214/215 (99%)	0.45	4 (1%) 66 48	30, 75, 96, 107	0
All	All	842/874 (96%)	0.57	40 (4%) 35 24	30, 72, 105, 129	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	82	VAL	3.9
1	G	115	VAL	3.3
1	G	376	CYS	3.0
2	H	137	ALA	2.9
3	L	137	ASN	2.9
2	H	41	PRO	2.9
2	H	10	GLU	2.7
2	H	112	SER	2.7
3	L	19	ALA	2.6
2	H	147	PRO	2.6
2	H	82(A)	SER	2.5
1	G	116	THR	2.5
1	G	163	ASP	2.5
1	G	239	VAL	2.4
2	H	198	VAL	2.4
1	G	309	ILE	2.4
1	G	383	PHE	2.4
2	H	17	SER	2.4
1	G	248	THR	2.4
1	G	26	PHE	2.3
1	G	10	TYR	2.3
3	L	62	PHE	2.3
1	G	158	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	367	THR	2.3
2	H	82(B)	ASN	2.2
1	G	160	ILE	2.2
2	H	15	GLY	2.2
2	H	135	THR	2.2
1	G	270	PRO	2.2
2	H	103	TRP	2.2
2	H	83	THR	2.2
1	G	289	GLY	2.2
3	L	83	PHE	2.1
2	H	105	LEU	2.1
1	G	292	ALA	2.1
1	G	156	THR	2.1
1	G	159	TYR	2.1
1	G	206	GLU	2.1
1	G	293	SER	2.0
1	G	57	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	503	14/15	0.66	0.29	16,17,18,18	0
4	NAG	G	506	14/15	0.67	0.26	26,27,29,30	0
4	NAG	G	505	14/15	0.68	0.30	25,26,27,27	0
4	NAG	G	507	14/15	0.71	0.21	19,20,21,24	0
4	NAG	G	501	14/15	0.72	0.21	5,6,9,9	0
4	NAG	G	504	14/15	0.74	0.26	22,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	502	14/15	0.74	0.28	7,7,8,9	0
4	NAG	G	508	14/15	0.81	0.15	24,24,26,26	0
5	GOL	G	509	6/6	0.82	0.09	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.