



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:15 AM UTC

PDB ID : 1DQD / pdb_00001dqd
Title : CRYSTAL STRUCTURE OF FAB HGR-2 F6, A COMPETITIVE ANTAGONIST OF THE GLUCAGON RECEPTOR
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Deposited on : 2000-01-04
Resolution : 2.10 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
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

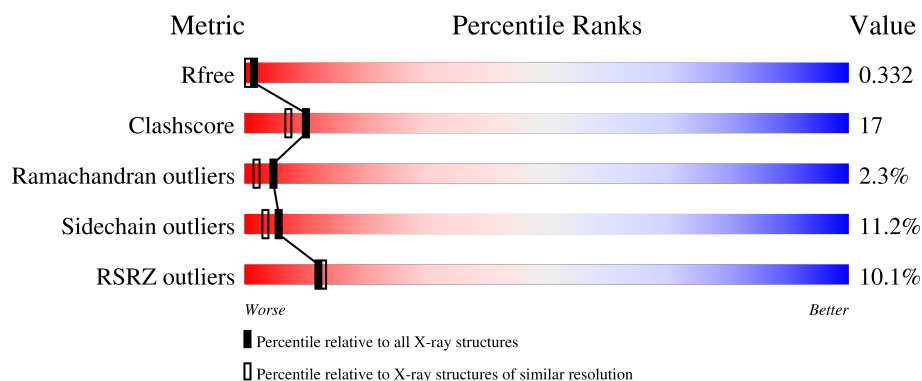
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	221	5% 59% 30% 5% .
2	H	222	14% 57% 33% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3699 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 HGR-2 F6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	4	6	0
			1643	1015	278	339	11			

- Molecule 2 is a protein called FAB HGR-2 F6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	1	0
			1676	1063	267	339	7			

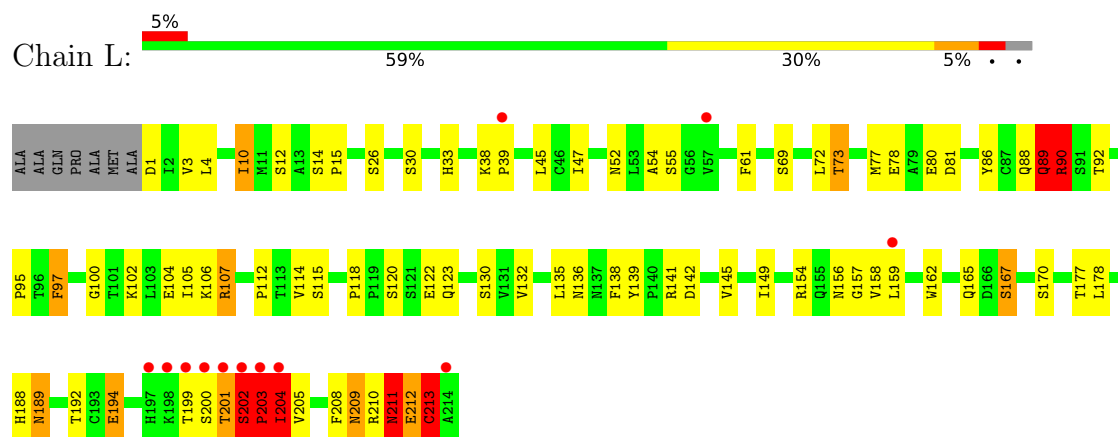
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	204	Total	O	0	0
			204	204		
3	H	176	Total	O	0	0
			176	176		

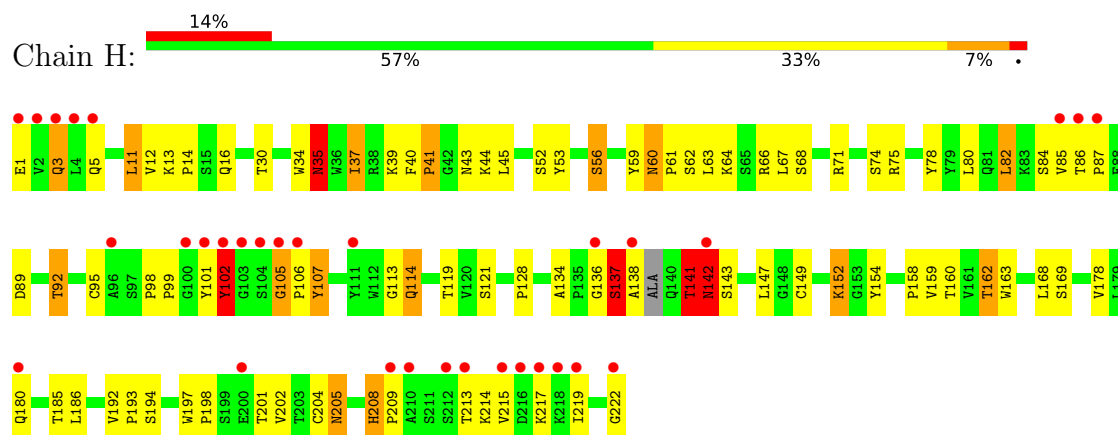
3 Residue-property plots [i](#)

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 HGR-2 F6



• Molecule 2: FAB HGR-2 F6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.14Å 133.74Å 37.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.10) 97.5 (20.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.315 0.234 , 0.332	Depositor DCC
R_{free} test set	2336 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	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	3699	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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](#)

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	1.18	3/1711 (0.2%)	1.73	40/2326 (1.7%)
2	H	0.63	1/1730 (0.1%)	1.86	37/2372 (1.6%)
All	All	0.95	4/3441 (0.1%)	1.80	77/4698 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	194	GLU	CD-OE1	-29.74	0.68	1.25
1	L	194	GLU	CD-OE2	21.49	1.66	1.25
1	L	12	SER	CA-CB	-21.46	1.04	1.53
2	H	142	ASN	N-CA	-6.65	1.37	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	141	THR	CA-C-N	25.21	169.69	121.54
2	H	141	THR	C-N-CA	25.21	169.69	121.54
2	H	208	HIS	CA-C-O	-16.99	103.44	120.09
2	H	141	THR	CA-C-O	14.53	138.83	121.68
1	L	194	GLU	CG-CD-OE2	-13.48	87.40	118.40
1	L	12	SER	N-CA-CB	-12.45	89.17	110.83
1	L	90	ARG	CD-NE-CZ	11.69	140.76	124.40
1	L	136	ASN	CA-CB-CG	10.71	123.31	112.60
2	H	141	THR	N-CA-C	10.01	125.12	109.81
2	H	141	THR	O-C-N	-9.31	109.62	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	35	ASN	CA-CB-CG	9.10	121.70	112.60
1	L	157	GLY	N-CA-C	-8.41	102.89	115.00
1	L	97	PHE	CA-CB-CG	8.27	122.07	113.80
2	H	142	ASN	N-CA-CB	8.13	124.23	110.49
1	L	211	ASN	CA-CB-CG	8.06	120.66	112.60
1	L	203	PRO	N-CA-C	8.06	129.07	112.47
2	H	66	ARG	NE-CZ-NH2	8.02	126.42	119.20
1	L	202	SER	CA-C-N	7.73	129.50	119.84
1	L	202	SER	C-N-CA	7.73	129.50	119.84
1	L	203	PRO	CA-C-N	7.52	135.51	121.97
1	L	203	PRO	C-N-CA	7.52	135.51	121.97
1	L	33	HIS	CA-CB-CG	-7.50	106.30	113.80
2	H	209	PRO	N-CA-CB	7.22	111.27	103.33
2	H	142	ASN	CA-C-N	7.18	132.09	120.60
2	H	142	ASN	C-N-CA	7.18	132.09	120.60
2	H	152	LYS	N-CA-C	7.06	121.17	109.95
2	H	107	TYR	N-CA-C	7.01	121.26	109.76
1	L	1	ASP	CA-CB-CG	-6.81	105.79	112.60
1	L	194	GLU	CG-CD-OE1	6.77	133.98	118.40
2	H	142	ASN	CA-CB-CG	-6.54	106.06	112.60
1	L	157	GLY	CA-C-O	6.53	126.21	118.97
2	H	209	PRO	CA-N-CD	-6.49	102.91	112.00
2	H	102	TYR	N-CA-C	6.43	124.51	110.80
2	H	71	ARG	CD-NE-CZ	6.37	133.31	124.40
2	H	92	THR	N-CA-CB	6.33	120.75	110.43
2	H	43	ASN	N-CA-C	6.20	120.42	112.86
1	L	213[A]	CYS	CA-C-O	6.15	129.30	120.51
1	L	213[B]	CYS	CA-C-O	6.15	129.30	120.51
1	L	12	SER	CB-CA-C	6.10	121.03	109.37
2	H	89	ASP	N-CA-C	-6.08	105.03	112.88
1	L	156	ASN	CA-C-O	6.06	129.17	120.51
2	H	201	THR	N-CA-C	6.03	118.80	110.35
2	H	141	THR	N-CA-CB	-6.02	102.02	111.05
1	L	115	SER	CA-CB-OG	6.01	123.11	111.10
1	L	203	PRO	CA-N-CD	-5.99	103.62	112.00
1	L	30	SER	CA-C-O	-5.97	114.09	120.42
2	H	208	HIS	CA-C-N	5.95	125.65	119.05
2	H	208	HIS	C-N-CA	5.95	125.65	119.05
2	H	102	TYR	CA-C-O	5.83	128.84	120.51
1	L	203	PRO	CA-C-O	5.70	130.96	120.60
1	L	203	PRO	N-CA-CB	-5.64	97.33	103.25
1	L	188	HIS	CA-CB-CG	-5.60	108.20	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	119	THR	CA-C-N	-5.60	115.50	123.11
2	H	119	THR	C-N-CA	-5.60	115.50	123.11
1	L	107	ARG	CD-NE-CZ	5.51	132.11	124.40
1	L	211	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	H	113	GLY	N-CA-C	-5.42	103.88	112.66
2	H	71	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	H	74	SER	CA-C-N	5.32	131.70	121.54
2	H	74	SER	C-N-CA	5.32	131.70	121.54
2	H	66	ARG	NE-CZ-NH1	-5.32	116.19	121.50
1	L	97	PHE	CA-C-O	5.31	127.11	121.11
1	L	189	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	H	41	PRO	N-CA-C	-5.20	103.03	111.03
1	L	61	PHE	CA-C-O	-5.18	115.61	121.72
1	L	90	ARG	CA-C-O	-5.14	113.82	119.78
1	L	114	VAL	CA-C-O	5.14	126.58	120.72
1	L	90	ARG	N-CA-C	-5.11	105.36	112.30
1	L	73	THR	N-CA-C	5.09	117.69	108.69
1	L	89	GLN	CA-CB-CG	5.08	124.26	114.10
1	L	100	GLY	N-CA-C	5.07	118.97	112.18
1	L	61	PHE	CA-CB-CG	5.04	118.84	113.80
2	H	143	SER	N-CA-C	5.02	118.51	112.38
1	L	52	ASN	CA-CB-CG	-5.01	107.59	112.60
2	H	84	SER	N-CA-CB	-5.01	104.09	111.71
2	H	102	TYR	CA-CB-CG	-5.01	104.88	113.90
1	L	69	SER	CA-C-O	5.01	126.56	120.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	208	HIS	Peptide,Mainchain

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	1643	0	1579	61	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1676	0	1618	58	0
3	H	176	0	0	6	0
3	L	204	0	0	3	0
All	All	3699	0	3197	112	1

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 17.

All (112) 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:L:141[A]:ARG:HH12	1:L:162:TRP:CD1	1.59	1.19
1:L:105:ILE:H	1:L:165:GLN:HE22	1.05	0.96
1:L:132:VAL:HG22	1:L:177[A]:THR:HG22	1.47	0.95
2:H:162:THR:HG23	2:H:205:ASN:HB2	1.48	0.94
1:L:38:LYS:HG2	1:L:39:PRO:HD2	1.51	0.90
1:L:141[A]:ARG:NH1	1:L:162:TRP:CD1	2.40	0.89
1:L:209:ASN:HD22	1:L:211:ASN:H	1.18	0.89
2:H:101:TYR:O	2:H:102:TYR:HB2	1.78	0.83
2:H:60:ASN:HD22	2:H:62:SER:H	1.32	0.78
2:H:86:THR:HB	2:H:87:PRO:HD2	1.65	0.77
1:L:89:GLN:HE22	1:L:92:THR:H	1.31	0.75
1:L:154:ARG:HD3	1:L:178:LEU:HD11	1.68	0.74
2:H:114:GLN:NE2	2:H:114:GLN:H	1.86	0.73
2:H:114:GLN:H	2:H:114:GLN:HE21	1.34	0.73
1:L:202:SER:N	1:L:203:PRO:HD2	2.08	0.69
1:L:209:ASN:ND2	1:L:211:ASN:H	1.91	0.66
1:L:105:ILE:N	1:L:165:GLN:HE22	1.88	0.66
2:H:60:ASN:ND2	2:H:62:SER:H	1.94	0.65
1:L:118:PRO:HB3	1:L:208:PHE:CE2	2.33	0.64
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.79	0.63
1:L:211:ASN:HD22	1:L:212:GLU:N	1.97	0.62
1:L:105:ILE:H	1:L:165:GLN:NE2	1.88	0.62
1:L:211:ASN:HD22	1:L:211:ASN:C	2.09	0.60
1:L:189:ASN:HB3	1:L:209:ASN:ND2	2.17	0.60
1:L:194:GLU:HG3	1:L:205:VAL:HG22	1.84	0.60
1:L:77:MET:HE3	1:L:81:ASP:HB2	1.85	0.59
1:L:3:VAL:H	1:L:26:SER:CB	2.15	0.59
1:L:189:ASN:HB3	1:L:209:ASN:HD21	1.68	0.58
2:H:180:GLN:HB3	3:H:244:HOH:O	2.02	0.57
2:H:147:LEU:HD12	2:H:202:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:VAL:H	1:L:26:SER:HB2	1.70	0.57
1:L:192:THR:HG23	1:L:205:VAL:HG13	1.87	0.57
1:L:123:GLN:HE22	1:L:130:SER:H	1.53	0.56
1:L:159:LEU:HD11	2:H:178:VAL:HB	1.87	0.56
1:L:77:MET:HE3	1:L:78:GLU:O	2.06	0.55
2:H:40:PHE:HB3	2:H:41:PRO:HD2	1.88	0.55
2:H:14:PRO:HA	2:H:85:VAL:O	2.07	0.55
2:H:35:ASN:C	2:H:35:ASN:HD22	2.15	0.55
1:L:86:TYR:OH	2:H:39:LYS:NZ	2.41	0.54
1:L:106:LYS:HA	1:L:139:TYR:OH	2.08	0.54
1:L:159:LEU:HB3	1:L:177[A]:THR:OG1	2.08	0.52
2:H:114:GLN:HE21	2:H:114:GLN:N	2.06	0.52
1:L:102:LYS:NZ	1:L:141[B]:ARG:HH12	2.08	0.52
1:L:72:LEU:C	1:L:72:LEU:HD23	2.34	0.52
1:L:149:ILE:HD11	1:L:154:ARG:HD2	1.92	0.51
2:H:192:VAL:HB	2:H:193:PRO:HD2	1.92	0.51
2:H:197:TRP:CG	2:H:198:PRO:HA	2.46	0.51
1:L:123:GLN:NE2	1:L:130:SER:H	2.08	0.51
2:H:80:LEU:HD23	2:H:80:LEU:C	2.36	0.50
1:L:120:SER:HB2	1:L:122:GLU:OE1	2.12	0.50
2:H:134:ALA:HB2	2:H:219:ILE:HG22	1.93	0.50
1:L:201:THR:O	1:L:202:SER:CB	2.61	0.49
2:H:106:PRO:HG2	2:H:107:TYR:CE1	2.47	0.49
2:H:141:THR:HG23	2:H:142:ASN:N	2.28	0.49
2:H:197:TRP:CD1	2:H:202:VAL:HG22	2.49	0.48
2:H:163:TRP:CH2	2:H:204:CYS:HB3	2.49	0.48
1:L:204:ILE:H	1:L:204:ILE:HD13	1.77	0.48
2:H:149:CYS:SG	2:H:219:ILE:HD11	2.53	0.48
1:L:135:LEU:HD21	1:L:145[A]:VAL:HG22	1.95	0.48
1:L:14:SER:HB3	1:L:15:PRO:HD2	1.95	0.48
2:H:40:PHE:CD1	2:H:44:LYS:HE2	2.49	0.48
2:H:178:VAL:HG23	3:H:258:HOH:O	2.13	0.48
2:H:34:TRP:HB3	2:H:78:TYR:CZ	2.49	0.47
2:H:82:LEU:HD13	2:H:85:VAL:HG12	1.96	0.47
1:L:72:LEU:HD23	1:L:73:THR:N	2.29	0.47
1:L:189:ASN:O	1:L:209:ASN:HA	2.15	0.47
2:H:136:GLY:O	2:H:137:SER:HB2	2.14	0.47
1:L:201:THR:O	1:L:202:SER:HB2	2.15	0.47
2:H:30:THR:O	2:H:53:TYR:HB2	2.15	0.47
2:H:213:THR:HG22	2:H:215:VAL:HG23	1.97	0.47
2:H:60:ASN:HB3	2:H:63:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:ILE:CD1	1:L:154:ARG:HD2	2.45	0.46
1:L:45:LEU:HD13	2:H:99:PRO:HG3	1.97	0.46
2:H:3:GLN:HB3	3:H:385:HOH:O	2.15	0.46
2:H:41:PRO:HB3	3:H:379:HOH:O	2.14	0.46
2:H:192:VAL:HB	2:H:193:PRO:CD	2.46	0.46
1:L:177[A]:THR:HG23	3:L:261:HOH:O	2.16	0.46
1:L:102:LYS:HZ1	1:L:141[B]:ARG:HH12	1.64	0.46
1:L:102:LYS:NZ	1:L:141[B]:ARG:NH1	2.64	0.45
1:L:90:ARG:HG2	1:L:95:PRO:HB3	1.98	0.45
2:H:16:GLN:O	2:H:85:VAL:HG22	2.17	0.45
1:L:167:SER:HB3	3:L:329:HOH:O	2.17	0.44
2:H:60:ASN:ND2	2:H:61:PRO:HD2	2.32	0.44
2:H:141:THR:HG23	2:H:142:ASN:HA	1.98	0.44
1:L:107:ARG:HD2	1:L:170:SER:HB2	2.00	0.44
2:H:138:ALA:HB2	3:H:383:HOH:O	2.16	0.44
2:H:62:SER:OG	2:H:63:LEU:HD22	2.18	0.44
1:L:88:GLN:HG2	1:L:89:GLN:N	2.32	0.44
1:L:97:PHE:CZ	2:H:37:ILE:HD13	2.53	0.44
1:L:122:GLU:OE2	2:H:217:LYS:HE3	2.18	0.44
1:L:158:VAL:HG22	1:L:178:LEU:HD13	2.00	0.43
1:L:159:LEU:HD23	1:L:159:LEU:O	2.18	0.43
2:H:13:LYS:H	2:H:16:GLN:NE2	2.16	0.43
1:L:54:ALA:O	1:L:55:SER:C	2.61	0.43
2:H:11:LEU:HD22	2:H:12:VAL:N	2.33	0.43
1:L:213[A]:CYS:SG	2:H:222:GLY:C	3.02	0.43
2:H:152:LYS:HB2	2:H:185:THR:HG23	2.01	0.42
1:L:10:ILE:HD13	1:L:10:ILE:O	2.20	0.42
2:H:60:ASN:HD22	2:H:61:PRO:N	2.18	0.42
2:H:101:TYR:O	2:H:102:TYR:CB	2.57	0.42
1:L:142:ASP:HB2	3:L:301:HOH:O	2.19	0.41
2:H:34:TRP:HB3	2:H:78:TYR:CE2	2.55	0.41
1:L:97:PHE:HZ	2:H:37:ILE:HD13	1.85	0.41
1:L:141[A]:ARG:HH12	1:L:162:TRP:CG	2.23	0.41
2:H:98:PRO:HG3	3:H:290:HOH:O	2.21	0.41
2:H:59:TYR:CZ	2:H:68:SER:HA	2.56	0.41
2:H:105:GLY:HA2	2:H:106:PRO:HD3	1.81	0.41
1:L:112:PRO:HA	1:L:138:PHE:HB3	2.02	0.40
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.21	0.40
2:H:141:THR:CG2	2:H:142:ASN:N	2.84	0.40
1:L:47:ILE:HD12	1:L:72:LEU:HD12	2.04	0.40
2:H:52:SER:OG	2:H:56:SER:N	2.54	0.40

All (1) 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:L:90:ARG:O	1:L:210:ARG:NH2[3_545]	1.87	0.33

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	218/221 (99%)	205 (94%)	8 (4%)	5 (2%)	5	2
2	H	218/222 (98%)	197 (90%)	15 (7%)	6 (3%)	4	1
All	All	436/443 (98%)	402 (92%)	23 (5%)	11 (2%)	5	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	SER
1	L	203	PRO
1	L	204	ILE
2	H	102	TYR
2	H	75	ARG
2	H	105	GLY
2	H	137	SER
1	L	213[A]	CYS
1	L	213[B]	CYS
2	H	142	ASN
2	H	64	LYS

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	194/191 (102%)	177 (91%)	17 (9%)	9	7
2	H	196/195 (100%)	169 (86%)	27 (14%)	3	2
All	All	390/386 (101%)	346 (89%)	44 (11%)	6	3

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	10	ILE
1	L	80	GLU
1	L	89	GLN
1	L	90	ARG
1	L	104	GLU
1	L	167	SER
1	L	199	THR
1	L	200	SER
1	L	201	THR
1	L	203	PRO
1	L	204	ILE
1	L	209	ASN
1	L	211	ASN
1	L	212	GLU
1	L	213[A]	CYS
1	L	213[B]	CYS
2	H	1	GLU
2	H	3	GLN
2	H	5	GLN
2	H	11	LEU
2	H	35	ASN
2	H	37	ILE
2	H	45	LEU
2	H	56	SER
2	H	60	ASN
2	H	67	LEU
2	H	82	LEU
2	H	92	THR
2	H	114	GLN
2	H	121	SER
2	H	137	SER
2	H	141	THR

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Mol	Chain	Res	Type
2	H	142	ASN
2	H	158	PRO
2	H	159	VAL
2	H	160	THR
2	H	162	THR
2	H	168	LEU
2	H	169	SER
2	H	186	LEU
2	H	194	SER
2	H	205	ASN
2	H	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	88	GLN
1	L	89	GLN
1	L	123	GLN
1	L	136	ASN
1	L	144	ASN
1	L	165	GLN
1	L	209	ASN
1	L	211	ASN
2	H	3	GLN
2	H	16	GLN
2	H	35	ASN
2	H	60	ASN
2	H	114	GLN
2	H	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

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	214/221 (96%)	0.47	12 (5%)	30 32	22, 36, 57, 95	14 (6%)
2	H	221/222 (99%)	0.89	32 (14%)	6 6	24, 42, 83, 99	12 (5%)
All	All	435/443 (98%)	0.69	44 (10%)	12 13	22, 39, 82, 99	26 (5%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	104	SER	5.3
2	H	219	ILE	5.0
2	H	2	VAL	4.6
2	H	217	LYS	4.4
2	H	1	GLU	4.3
2	H	105	GLY	4.3
1	L	204	ILE	4.3
2	H	102	TYR	4.2
1	L	199	THR	4.1
1	L	203	PRO	3.8
2	H	222	GLY	3.6
1	L	198	LYS	3.6
1	L	201	THR	3.4
2	H	215	VAL	3.3
2	H	138	ALA	3.2
2	H	213	THR	3.2
2	H	101	TYR	3.1
2	H	106	PRO	3.0
2	H	96	ALA	3.0
1	L	159	LEU	3.0
1	L	200	SER	2.6
2	H	85	VAL	2.6
2	H	100	GLY	2.5
2	H	4	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	103	GLY	2.5
1	L	202	SER	2.4
1	L	197	HIS	2.4
1	L	214	ALA	2.3
2	H	210	ALA	2.3
2	H	216	ASP	2.3
2	H	200	GLU	2.3
2	H	3	GLN	2.3
2	H	87	PRO	2.3
2	H	209	PRO	2.2
2	H	218	LYS	2.2
2	H	86	THR	2.2
2	H	5	GLN	2.1
2	H	111	TYR	2.1
1	L	39	PRO	2.1
2	H	212	SER	2.1
2	H	142	ASN	2.1
2	H	136	GLY	2.1
1	L	57	VAL	2.0
2	H	180	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.