



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:50 PM UTC

PDB ID : 2NRF / pdb_00002nrf
Title : Crystal Structure of GlpG, a Rhomboid family intramembrane protease
Authors : Wu, Z.; Yan, N.; Feng, L.; Yan, H.; Gu, L.; Shi, Y.
Deposited on : 2006-11-02
Resolution : 2.60 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

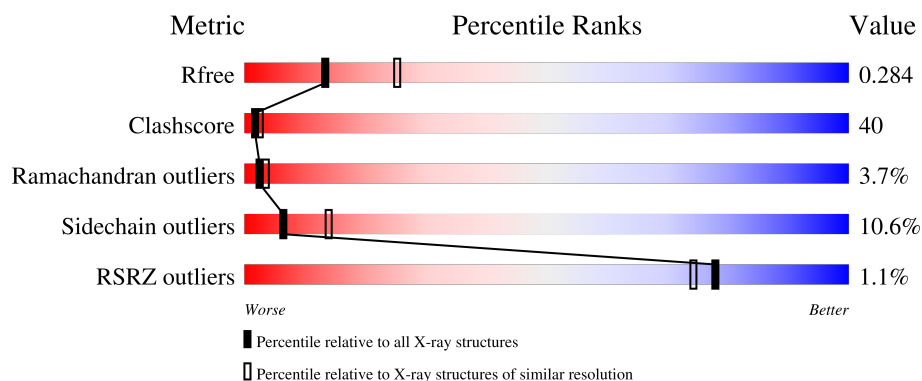
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	182	2% 42% 43% 15% .
1	B	182	% 41% 43% 10% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2861 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 Protein GlpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1452	978	232	231	11			
1	B	173	Total	C	N	O	S	0	0	0
			1383	932	223	219	9			

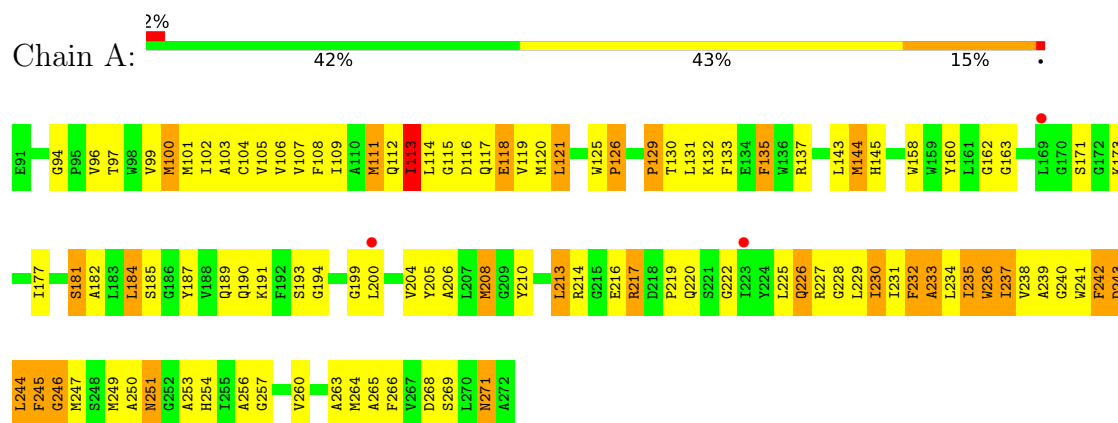
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	17	Total	O	0	0
			17	17		

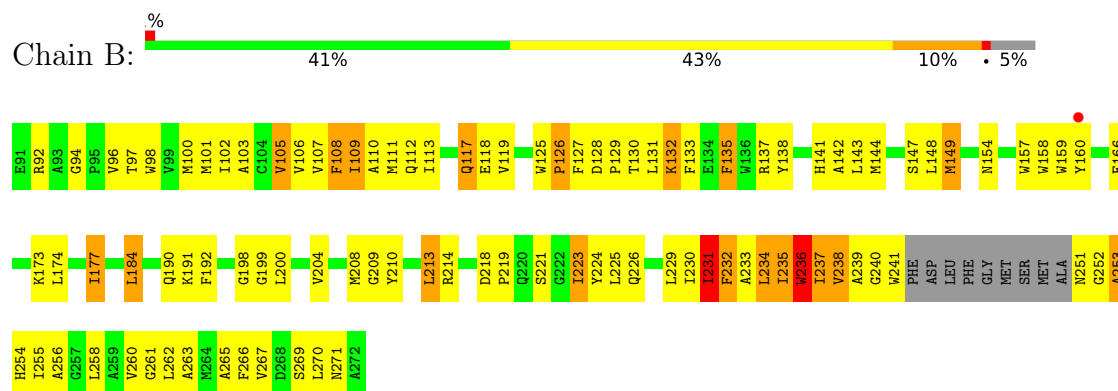
3 Residue-property plots

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: Protein GlpG



• Molecule 1: Protein GlpG



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	59.46Å 59.46Å 118.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.60 51.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (100.00-2.60) 96.0 (51.49-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.262 , 0.295 0.262 , 0.284	Depositor DCC
R_{free} test set	1263 reflections (8.92%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 221.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.104 for -h,-k,l 0.418 for h,-h-k,-l 0.109 for -k,-h,-l	Xtriage
Reported twinning fraction	0.400 for h,-h-k,-l	Depositor
Outliers	0 of 14159 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2861	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

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	1.02	7/1501 (0.5%)	1.32	16/2041 (0.8%)
1	B	0.95	3/1429 (0.2%)	1.33	16/1944 (0.8%)
All	All	0.99	10/2930 (0.3%)	1.32	32/3985 (0.8%)

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
1	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	ALA	N-CA	-6.10	1.38	1.46
1	A	111	MET	CA-C	-5.99	1.45	1.52
1	A	264	MET	SD-CE	-5.75	1.65	1.79
1	B	110	ALA	CA-CB	-5.61	1.44	1.53
1	A	208	MET	SD-CE	-5.56	1.65	1.79
1	A	181	SER	CA-C	5.42	1.60	1.52
1	A	100	MET	SD-CE	5.35	1.93	1.79
1	B	263	ALA	CA-CB	-5.32	1.45	1.53
1	A	230	ILE	CA-CB	5.26	1.60	1.54
1	A	208	MET	CG-SD	5.14	1.93	1.80

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	PHE	N-CA-C	-11.48	99.29	113.18
1	A	235	ILE	N-CA-C	-10.90	97.46	111.09
1	B	105	VAL	N-CA-C	-10.05	101.07	110.82
1	A	230	ILE	N-CA-C	-8.64	101.29	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	TRP	N-CA-C	-8.27	102.97	113.72
1	A	237	ILE	N-CA-C	-8.23	100.81	111.09
1	B	234	LEU	N-CA-C	-7.93	103.06	112.89
1	B	238	VAL	N-CA-C	-7.80	105.11	112.83
1	A	135	PHE	N-CA-C	7.47	120.30	111.71
1	B	231	ILE	N-CA-C	7.42	120.18	112.83
1	B	135	PHE	N-CA-C	6.99	120.70	111.75
1	B	253	ALA	N-CA-C	-6.76	105.01	113.20
1	A	232	PHE	N-CA-C	-6.62	105.95	112.97
1	A	251	ASN	N-CA-C	6.62	120.27	110.48
1	A	181	SER	CA-C-N	6.35	129.31	120.29
1	A	181	SER	C-N-CA	6.35	129.31	120.29
1	B	108	PHE	N-CA-C	-6.33	103.67	111.33
1	B	261	GLY	N-CA-C	-6.24	105.09	112.64
1	A	269	SER	N-CA-C	-6.23	105.55	113.02
1	B	269	SER	N-CA-C	-6.17	106.01	112.93
1	B	192	PHE	N-CA-C	6.08	120.86	113.38
1	A	118	GLU	N-CA-C	6.07	118.39	111.11
1	A	253	ALA	N-CA-C	6.02	120.23	113.01
1	B	132	LYS	N-CA-C	5.99	119.41	111.75
1	B	235	ILE	N-CA-C	-5.90	104.99	113.07
1	B	237	ILE	N-CA-C	-5.68	105.56	111.58
1	B	177	ILE	CB-CA-C	-5.66	104.63	112.04
1	A	236	TRP	N-CA-C	5.47	118.42	111.69
1	A	250	ALA	N-CA-C	-5.36	99.38	110.80
1	A	182	ALA	N-CA-C	-5.33	105.55	111.36
1	A	233	ALA	N-CA-C	-5.23	99.67	110.80
1	A	144	MET	N-CA-C	5.04	118.02	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	138	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1452	0	1455	130	0
1	B	1383	0	1390	103	0
2	A	9	0	0	0	0
2	B	17	0	0	0	0
All	All	2861	0	2845	229	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 40.

All (229) 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:231:ILE:HG22	1:A:235:ILE:HG13	1.27	1.11
1:B:106:VAL:HA	1:B:109:ILE:HG12	1.15	1.10
1:A:239:ALA:HA	1:A:243:ASP:HB3	1.32	1.10
1:A:190:GLN:HA	1:A:194:GLY:O	1.52	1.08
1:A:237:ILE:O	1:A:241:TRP:HB3	1.55	1.04
1:B:106:VAL:HA	1:B:109:ILE:CG1	1.88	1.04
1:A:109:ILE:O	1:A:113:ILE:HG13	1.58	1.02
1:B:106:VAL:CA	1:B:109:ILE:HG12	1.92	1.00
1:A:97:THR:HG22	1:A:101:MET:HE2	1.45	0.97
1:B:234:LEU:HA	1:B:237:ILE:HD12	1.43	0.96
1:B:251:ASN:HD22	1:B:253:ALA:H	1.13	0.96
1:A:227:ARG:O	1:A:231:ILE:HG12	1.66	0.94
1:B:230:ILE:HG22	1:B:231:ILE:HD13	1.50	0.90
1:B:235:ILE:O	1:B:239:ALA:HB2	1.73	0.88
1:B:208:MET:HE2	1:B:233:ALA:HB1	1.55	0.87
1:A:231:ILE:CG2	1:A:235:ILE:HG13	2.06	0.85
1:A:105:VAL:O	1:A:109:ILE:HG13	1.78	0.83
1:A:238:VAL:HG22	1:A:241:TRP:CZ3	2.14	0.82
1:A:231:ILE:HG22	1:A:235:ILE:CG1	2.08	0.80
1:A:239:ALA:CA	1:A:243:ASP:HB3	2.12	0.79
1:A:244:LEU:HD23	1:A:245:PHE:N	1.98	0.79
1:B:234:LEU:HD23	1:B:234:LEU:O	1.82	0.78
1:A:160:TYR:CZ	1:A:229:LEU:HD13	2.18	0.78
1:B:126:PRO:HD3	1:B:137:ARG:HB3	1.65	0.77
1:B:129:PRO:O	1:B:132:LYS:HG2	1.85	0.76
1:A:204:VAL:O	1:A:208:MET:HG3	1.86	0.75
1:A:238:VAL:HG22	1:A:241:TRP:HZ3	1.48	0.75
1:B:98:TRP:HA	1:B:101:MET:HE3	1.68	0.75
1:B:154:ASN:ND2	1:B:236:TRP:HH2	1.85	0.74
1:A:242:PHE:C	1:A:244:LEU:H	1.95	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ALA:O	1:B:237:ILE:HG13	1.87	0.74
1:B:125:TRP:NE1	1:B:190:GLN:HG3	2.02	0.74
1:B:236:TRP:HA	1:B:239:ALA:HB2	1.70	0.73
1:A:239:ALA:HA	1:A:243:ASP:CB	2.13	0.72
1:B:173:LYS:O	1:B:177:ILE:HG13	1.89	0.72
1:B:251:ASN:ND2	1:B:253:ALA:H	1.86	0.72
1:B:208:MET:CE	1:B:233:ALA:HB1	2.20	0.71
1:B:232:PHE:C	1:B:235:ILE:HG22	2.16	0.70
1:B:97:THR:HG22	1:B:101:MET:HE2	1.72	0.70
1:A:225:LEU:HD22	1:A:230:ILE:N	2.05	0.70
1:A:200:LEU:O	1:A:204:VAL:HG23	1.90	0.70
1:B:154:ASN:ND2	1:B:236:TRP:CH2	2.61	0.68
1:A:99:VAL:O	1:A:102:ILE:HG22	1.93	0.68
1:A:235:ILE:O	1:A:239:ALA:HB2	1.94	0.68
1:A:133:PHE:CD2	1:A:135:PHE:CZ	2.83	0.66
1:B:157:TRP:HE1	1:B:236:TRP:CD1	2.13	0.66
1:A:109:ILE:O	1:A:112:GLN:HB2	1.96	0.65
1:A:235:ILE:O	1:A:239:ALA:CB	2.43	0.65
1:A:225:LEU:HB3	1:A:230:ILE:HG12	1.78	0.65
1:B:128:ASP:OD1	1:B:129:PRO:HD2	1.97	0.65
1:B:251:ASN:ND2	1:B:252:GLY:N	2.44	0.65
1:A:181:SER:O	1:A:185:SER:OG	2.12	0.64
1:B:208:MET:HE2	1:B:233:ALA:CB	2.27	0.64
1:A:118:GLU:OE1	1:A:121:LEU:HD23	1.98	0.64
1:A:213:LEU:CD2	1:A:217:ARG:HD2	2.28	0.63
1:B:107:VAL:HG11	1:B:143:LEU:O	1.99	0.62
1:A:129:PRO:O	1:A:132:LYS:HG2	1.99	0.62
1:B:233:ALA:HA	1:B:236:TRP:HB2	1.80	0.62
1:A:111:MET:O	1:A:112:GLN:C	2.42	0.62
1:A:121:LEU:HD12	1:A:121:LEU:O	2.01	0.61
1:A:230:ILE:O	1:A:233:ALA:HB3	2.01	0.60
1:A:238:VAL:HG13	1:A:242:PHE:HB2	1.83	0.60
1:A:225:LEU:HB3	1:A:230:ILE:CG1	2.31	0.60
1:A:271:ASN:HD22	1:B:191:LYS:HE3	1.65	0.60
1:B:236:TRP:HA	1:B:239:ALA:CB	2.31	0.60
1:A:113:ILE:C	1:A:115:GLY:H	2.10	0.60
1:A:190:GLN:NE2	1:A:191:LYS:N	2.49	0.60
1:A:121:LEU:HD12	1:A:121:LEU:C	2.27	0.59
1:B:251:ASN:O	1:B:254:HIS:HB2	2.03	0.59
1:B:184:LEU:HD13	1:B:256:ALA:HB1	1.84	0.59
1:B:234:LEU:HA	1:B:237:ILE:CD1	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:HIS:HA	1:B:144:MET:HE2	1.85	0.58
1:A:260:VAL:O	1:A:263:ALA:HB3	2.03	0.58
1:B:234:LEU:CA	1:B:237:ILE:HD12	2.25	0.58
1:A:100:MET:HG2	1:A:158:TRP:CZ2	2.39	0.57
1:A:187:TYR:HH	1:B:173:LYS:HZ3	1.48	0.57
1:B:251:ASN:ND2	1:B:252:GLY:H	2.02	0.57
1:B:148:LEU:HB3	1:B:149:MET:HE3	1.85	0.57
1:B:218:ASP:CG	1:B:221:SER:HB3	2.30	0.57
1:A:133:PHE:CE2	1:A:135:PHE:HZ	2.23	0.56
1:B:231:ILE:O	1:B:235:ILE:HB	2.04	0.56
1:A:187:TYR:OH	1:B:173:LYS:NZ	2.28	0.56
1:A:231:ILE:C	1:A:233:ALA:H	2.13	0.56
1:A:234:LEU:HD23	1:A:237:ILE:CG2	2.36	0.56
1:A:96:VAL:CG2	1:A:171:SER:HB3	2.36	0.55
1:A:213:LEU:HD21	1:A:217:ARG:HD2	1.88	0.55
1:A:238:VAL:HG12	1:A:238:VAL:O	2.05	0.55
1:A:234:LEU:HD23	1:A:237:ILE:HG22	1.88	0.55
1:B:117:GLN:HA	1:B:117:GLN:OE1	2.06	0.55
1:A:111:MET:HE2	1:A:116:ASP:OD1	2.07	0.55
1:A:238:VAL:CG1	1:A:242:PHE:HB2	2.36	0.55
1:B:147:SER:HB2	1:B:149:MET:SD	2.47	0.55
1:B:208:MET:HE1	1:B:236:TRP:HB3	1.89	0.55
1:A:113:ILE:C	1:A:115:GLY:N	2.63	0.55
1:B:230:ILE:CG2	1:B:231:ILE:HD13	2.30	0.55
1:A:118:GLU:O	1:A:121:LEU:HB3	2.08	0.54
1:B:200:LEU:O	1:B:204:VAL:HG23	2.07	0.54
1:B:100:MET:HG2	1:B:158:TRP:CE2	2.43	0.54
1:A:108:PHE:O	1:A:112:GLN:HG2	2.07	0.54
1:A:184:LEU:HD12	1:A:260:VAL:CG2	2.38	0.54
1:A:243:ASP:O	1:A:244:LEU:O	2.25	0.53
1:B:225:LEU:HD22	1:B:230:ILE:HA	1.89	0.53
1:A:160:TYR:CE2	1:A:229:LEU:HD13	2.43	0.53
1:B:160:TYR:CZ	1:B:229:LEU:HD12	2.43	0.53
1:A:225:LEU:HD22	1:A:230:ILE:CA	2.38	0.53
1:B:251:ASN:HD22	1:B:253:ALA:N	1.95	0.52
1:B:106:VAL:C	1:B:109:ILE:HG12	2.33	0.52
1:B:142:ALA:HA	1:B:199:GLY:O	2.09	0.52
1:A:245:PHE:O	1:A:246:GLY:O	2.28	0.52
1:A:213:LEU:HD22	1:A:217:ARG:HD2	1.91	0.52
1:A:249:MET:O	1:A:251:ASN:N	2.42	0.52
1:A:102:ILE:HG23	1:A:103:ALA:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:HZ2	1:A:268:ASP:CG	2.18	0.51
1:A:249:MET:O	1:A:249:MET:SD	2.68	0.51
1:B:97:THR:O	1:B:101:MET:HE2	2.11	0.51
1:B:106:VAL:O	1:B:109:ILE:HB	2.11	0.51
1:A:120:MET:O	1:A:121:LEU:C	2.54	0.50
1:B:125:TRP:CD1	1:B:190:GLN:HG3	2.46	0.50
1:A:235:ILE:O	1:A:239:ALA:N	2.44	0.50
1:B:240:GLY:O	1:B:241:TRP:HE3	1.95	0.50
1:B:232:PHE:O	1:B:235:ILE:HG22	2.11	0.50
1:A:109:ILE:O	1:A:113:ILE:CG1	2.45	0.49
1:B:154:ASN:HD21	1:B:236:TRP:HH2	1.55	0.49
1:B:238:VAL:HG12	1:B:238:VAL:O	2.11	0.49
1:A:100:MET:HG2	1:A:158:TRP:CE2	2.47	0.49
1:A:111:MET:O	1:A:115:GLY:N	2.45	0.49
1:B:96:VAL:CG1	1:B:174:LEU:HD23	2.42	0.49
1:B:133:PHE:O	1:B:135:PHE:CD2	2.65	0.49
1:B:252:GLY:C	1:B:254:HIS:H	2.20	0.49
1:A:144:MET:O	1:A:199:GLY:N	2.46	0.49
1:A:126:PRO:HD3	1:A:137:ARG:CB	2.43	0.49
1:A:97:THR:HG22	1:A:101:MET:CE	2.30	0.48
1:A:229:LEU:O	1:A:230:ILE:C	2.56	0.48
1:A:238:VAL:HG22	1:A:241:TRP:CE3	2.46	0.48
1:B:148:LEU:CB	1:B:149:MET:HE3	2.43	0.48
1:B:266:PHE:O	1:B:270:LEU:HB2	2.13	0.48
1:B:157:TRP:CH2	1:B:233:ALA:HB2	2.48	0.48
1:A:102:ILE:CG2	1:A:103:ALA:N	2.77	0.48
1:B:106:VAL:O	1:B:106:VAL:HG12	2.13	0.48
1:A:220:GLN:C	1:A:222:GLY:N	2.68	0.48
1:B:210:TYR:HA	1:B:265:ALA:HB2	1.96	0.48
1:A:217:ARG:NH2	1:A:266:PHE:HE1	2.11	0.47
1:A:226:GLN:HB2	1:A:229:LEU:HD12	1.95	0.47
1:A:190:GLN:CD	1:A:191:LYS:N	2.72	0.47
1:A:231:ILE:HG22	1:A:235:ILE:CD1	2.43	0.47
1:B:234:LEU:HA	1:B:237:ILE:HB	1.97	0.47
1:B:267:VAL:O	1:B:270:LEU:HB3	2.14	0.47
1:A:173:LYS:O	1:A:177:ILE:HG13	2.15	0.47
1:B:231:ILE:HG23	1:B:234:LEU:HB3	1.97	0.47
1:B:102:ILE:CG2	1:B:103:ALA:N	2.77	0.47
1:B:111:MET:HG3	1:B:119:VAL:HG21	1.97	0.47
1:A:205:TYR:CE1	1:A:254:HIS:ND1	2.82	0.47
1:A:234:LEU:O	1:A:238:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASP:O	1:A:243:ASP:OD1	2.32	0.46
1:A:113:ILE:HG21	1:A:113:ILE:HD13	1.48	0.46
1:A:236:TRP:N	1:A:236:TRP:CD1	2.81	0.46
1:B:231:ILE:HG23	1:B:234:LEU:HD13	1.98	0.46
1:A:96:VAL:HG23	1:A:171:SER:HB3	1.98	0.46
1:A:184:LEU:HD13	1:A:256:ALA:HB1	1.97	0.46
1:B:209:GLY:O	1:B:213:LEU:HB2	2.16	0.46
1:A:162:GLY:O	1:A:163:GLY:C	2.58	0.46
1:A:226:GLN:CB	1:A:229:LEU:HD12	2.46	0.46
1:B:94:GLY:HA3	1:B:166:GLU:CD	2.41	0.46
1:B:127:PHE:CE1	1:B:131:LEU:HD13	2.51	0.46
1:A:111:MET:HA	1:A:119:VAL:HG21	1.97	0.46
1:A:113:ILE:O	1:A:115:GLY:N	2.49	0.46
1:A:190:GLN:CD	1:A:190:GLN:C	2.84	0.46
1:A:100:MET:CB	1:A:158:TRP:CZ2	3.00	0.45
1:A:242:PHE:O	1:A:244:LEU:N	2.49	0.45
1:A:102:ILE:O	1:A:106:VAL:HG23	2.16	0.45
1:A:111:MET:O	1:A:115:GLY:CA	2.64	0.45
1:A:97:THR:O	1:A:101:MET:HG3	2.17	0.45
1:A:210:TYR:HA	1:A:265:ALA:HB2	1.99	0.45
1:A:217:ARG:HH21	1:A:266:PHE:HE1	1.65	0.45
1:B:252:GLY:C	1:B:254:HIS:N	2.74	0.45
1:B:209:GLY:O	1:B:262:LEU:HD23	2.17	0.44
1:B:231:ILE:H	1:B:231:ILE:HG12	1.43	0.44
1:B:235:ILE:O	1:B:239:ALA:CB	2.56	0.44
1:A:245:PHE:HB3	1:A:246:GLY:H	1.56	0.44
1:A:217:ARG:O	1:A:219:PRO:HD3	2.18	0.44
1:B:233:ALA:C	1:B:236:TRP:H	2.26	0.44
1:A:108:PHE:CZ	1:A:112:GLN:NE2	2.86	0.44
1:B:108:PHE:O	1:B:112:GLN:HG2	2.17	0.44
1:A:189:GLN:O	1:A:190:GLN:C	2.60	0.44
1:B:125:TRP:HE1	1:B:190:GLN:HG3	1.78	0.44
1:A:126:PRO:HD3	1:A:137:ARG:HB3	1.99	0.43
1:B:125:TRP:O	1:B:126:PRO:C	2.60	0.43
1:A:256:ALA:O	1:A:260:VAL:HG23	2.19	0.43
1:A:133:PHE:CD2	1:A:135:PHE:HZ	2.33	0.43
1:A:158:TRP:O	1:A:162:GLY:N	2.52	0.43
1:A:96:VAL:HG21	1:A:171:SER:HB3	2.00	0.43
1:A:225:LEU:CD2	1:A:229:LEU:HB3	2.49	0.43
1:A:231:ILE:O	1:A:235:ILE:N	2.37	0.43
1:B:126:PRO:HD3	1:B:137:ARG:CB	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASN:ND2	1:B:191:LYS:HE3	2.33	0.43
1:A:220:GLN:C	1:A:222:GLY:H	2.25	0.42
1:A:227:ARG:O	1:A:231:ILE:CG1	2.54	0.42
1:B:105:VAL:HG12	1:B:109:ILE:HD11	2.01	0.42
1:A:100:MET:HB3	1:A:158:TRP:CZ2	2.53	0.42
1:A:111:MET:HE1	1:A:145:HIS:O	2.19	0.42
1:B:102:ILE:HG23	1:B:103:ALA:N	2.35	0.42
1:A:125:TRP:O	1:A:126:PRO:C	2.61	0.42
1:B:100:MET:HG2	1:B:158:TRP:CZ2	2.55	0.42
1:A:103:ALA:O	1:A:107:VAL:HG23	2.20	0.42
1:A:230:ILE:HG22	1:A:234:LEU:HD12	2.02	0.41
1:B:256:ALA:O	1:B:260:VAL:HG23	2.19	0.41
1:B:141:HIS:O	1:B:198:GLY:HA2	2.20	0.41
1:B:234:LEU:HD23	1:B:238:VAL:HG23	2.02	0.41
1:A:232:PHE:CD2	1:A:235:ILE:HD12	2.55	0.41
1:A:249:MET:O	1:A:249:MET:CG	2.68	0.41
1:B:106:VAL:HA	1:B:109:ILE:HG13	1.91	0.41
1:B:127:PHE:CE1	1:B:131:LEU:CD1	3.03	0.41
1:B:234:LEU:O	1:B:238:VAL:HG23	2.21	0.41
1:A:104:CYS:SG	1:A:200:LEU:HD22	2.61	0.41
1:A:244:LEU:HD23	1:A:245:PHE:H	1.80	0.41
1:A:244:LEU:HD23	1:A:245:PHE:O	2.21	0.41
1:B:160:TYR:CE2	1:B:229:LEU:HD12	2.55	0.41
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.75	0.41
1:A:225:LEU:O	1:A:230:ILE:HG13	2.21	0.41
1:A:228:GLY:O	1:A:231:ILE:HB	2.21	0.41
1:B:100:MET:CB	1:B:158:TRP:CZ2	3.03	0.41
1:A:113:ILE:HB	1:A:114:LEU:H	1.63	0.41
1:B:255:ILE:O	1:B:258:LEU:HB3	2.21	0.41
1:B:148:LEU:HA	1:B:148:LEU:HD12	1.82	0.41
1:B:160:TYR:CE2	1:B:229:LEU:CD1	3.03	0.41
1:A:236:TRP:HA	1:A:239:ALA:HB3	2.03	0.40
1:B:224:TYR:CD1	1:B:224:TYR:C	2.99	0.40
1:A:206:ALA:HB2	1:A:257:GLY:O	2.20	0.40
1:B:223:ILE:O	1:B:223:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

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	180/182 (99%)	148 (82%)	24 (13%)	8 (4%)	2	2
1	B	169/182 (93%)	151 (89%)	13 (8%)	5 (3%)	3	6
All	All	349/364 (96%)	299 (86%)	37 (11%)	13 (4%)	2	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	244	LEU
1	A	245	PHE
1	A	246	GLY
1	A	94	GLY
1	A	240	GLY
1	A	243	ASP
1	B	126	PRO
1	B	271	ASN
1	A	271	ASN
1	B	109	ILE
1	B	113	ILE
1	B	219	PRO

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	145/145 (100%)	128 (88%)	17 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	138/145 (95%)	125 (91%)	13 (9%)	8	18
All	All	283/290 (98%)	253 (89%)	30 (11%)	6	14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ILE
1	A	117	GLN
1	A	121	LEU
1	A	126	PRO
1	A	129	PRO
1	A	130	THR
1	A	131	LEU
1	A	143	LEU
1	A	184	LEU
1	A	193	SER
1	A	213	LEU
1	A	214	ARG
1	A	216	GLU
1	A	217	ARG
1	A	226	GLN
1	A	242	PHE
1	A	247	MET
1	B	92	ARG
1	B	117	GLN
1	B	118	GLU
1	B	130	THR
1	B	149	MET
1	B	159	TRP
1	B	184	LEU
1	B	213	LEU
1	B	214	ARG
1	B	223	ILE
1	B	226	GLN
1	B	231	ILE
1	B	236	TRP

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

Mol	Chain	Res	Type
1	A	145	HIS

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Mol	Chain	Res	Type
1	A	190	GLN
1	A	271	ASN
1	B	154	ASN
1	B	190	GLN
1	B	251	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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	182/182 (100%)	-0.20	3 (1%) 70 66	30, 88, 134, 158	0
1	B	173/182 (95%)	-0.20	1 (0%) 85 83	37, 98, 156, 162	0
All	All	355/364 (97%)	-0.20	4 (1%) 78 74	30, 94, 149, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	LEU	3.2
1	A	223	ILE	2.8
1	B	160	TYR	2.3
1	A	200	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.