Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NRF
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

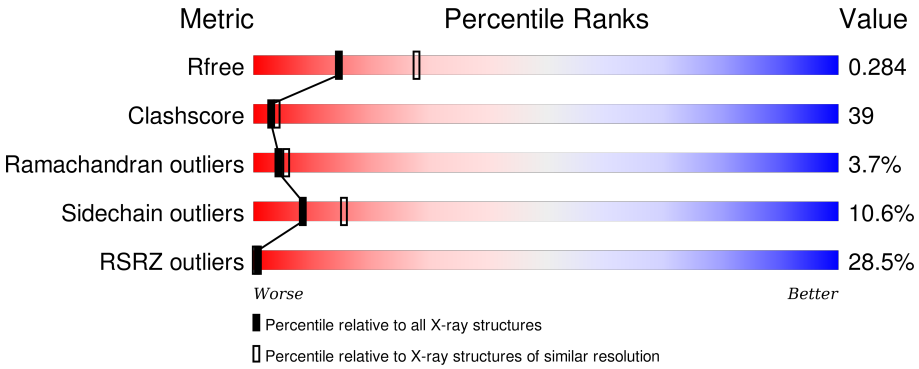
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	24% 47% 44% 8%
1	B	182	31% 43% 46% 5% 5%

2 Entry composition (i)

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.

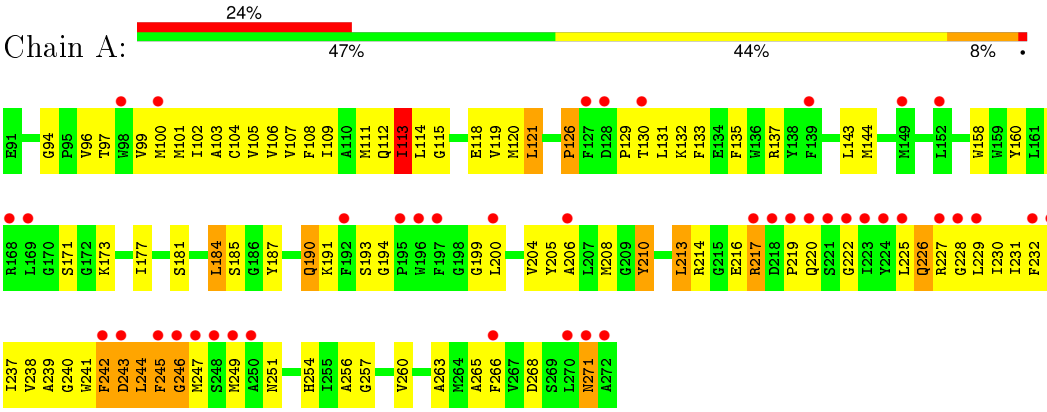
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	17	Total	O	0	0
			17	17		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

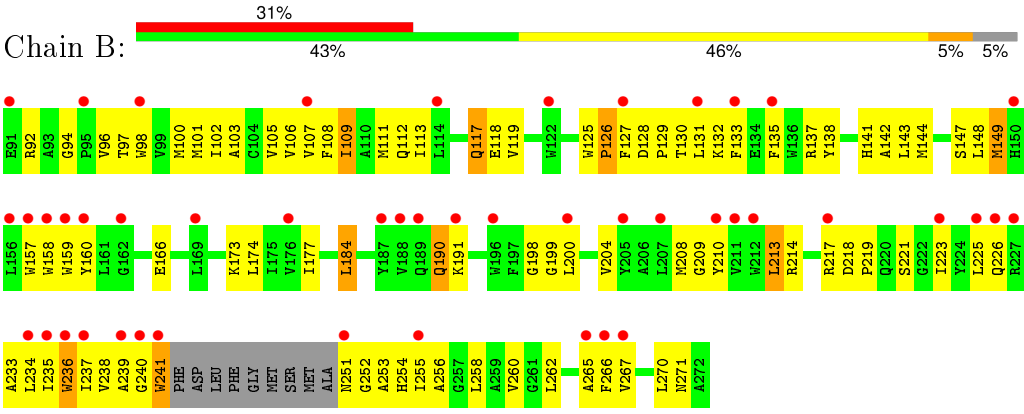
- Molecule 1: Protein GlpG

Chain A:



- Molecule 1: Protein GlpG

Chain B:



4 Data and refinement statistics (i)

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 47.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (100.00-2.60) 95.9 (47.20-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.262 , 0.295 0.263 , 0.284	Depositor DCC
R_{free} test set	1263 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 94.8	EDS
Estimated twinning fraction	0.104 for -h,-k,l 0.418 for h,-h-k,-l 0.109 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 14159 reflections	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.81	1/1501 (0.1%)	0.92	2/2041 (0.1%)
1	B	0.77	0/1429	0.84	0/1944
All	All	0.80	1/2930 (0.0%)	0.88	2/3985 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	TYR	CD1-CE1	5.28	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ILE	CG1-CB-CG2	-6.66	96.75	111.40
1	A	235	ILE	N-CA-C	-5.01	97.46	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1452	0	1455	127	0
1	B	1383	0	1390	97	0
2	A	9	0	0	0	0
2	B	17	0	0	0	0
All	All	2861	0	2845	220	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 39.

All (220) 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: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: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:B:97:THR:O	1:B:101:MET:HE2	1.81	0.81
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:O	1:B:234:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:ASN:ND2	1:B:236:TRP:HH2	1.85	0.74
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: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:242:PHE:C	1:A:244:LEU:H	1.95	0.68
1:A:133:PHE:CD2	1:A:135:PHE:CZ	2.83	0.66
1:B:232:PHE:C	1:B:235:ILE:HG22	2.16	0.66
1:A:235:ILE:O	1:A:239:ALA:CB	2.43	0.65
1:A:109:ILE:O	1:A:112:GLN:HB2	1.96	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:A:118:GLU:OE1	1:A:121:LEU:HD23	1.98	0.64
1:A:97:THR:HG22	1:A:101:MET:HE2	1.81	0.63
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:121:LEU:O	1:A:121:LEU:HD12	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:B:236:TRP:HA	1:B:239:ALA:CB	2.31	0.60
1:A:271:ASN:HD22	1:B:191:LYS:HE3	1.65	0.60
1:A:190:GLN:NE2	1:A:191:LYS:N	2.49	0.60
1:A:97:THR:HG22	1:A:101:MET:CE	2.30	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HA	1:B:237:ILE:CD1	2.26	0.59
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:B:251:ASN:ND2	1:B:252:GLY:H	2.02	0.57
1:A:111:MET:O	1:A:112:GLN:C	2.42	0.57
1:A:187:TYR:HH	1:B:173:LYS:HZ3	1.48	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:234:LEU:HD23	1:A:237:ILE:CG2	2.36	0.56
1:A:213:LEU:HD21	1:A:217:ARG:HD2	1.88	0.55
1:A:96:VAL:CG2	1:A:171:SER:HB3	2.36	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:A:113:ILE:C	1:A:115:GLY:H	2.10	0.55
1:B:117:GLN:OE1	1:B:117:GLN:HA	2.06	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:230:ILE:CG2	1:B:231:ILE:HD13	2.30	0.55
1:A:121:LEU:C	1:A:121:LEU:HD12	2.27	0.54
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:142:ALA:HA	1:B:199:GLY:O	2.09	0.52
1:A:231:ILE:C	1:A:233:ALA:H	2.13	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:113:ILE:C	1:A:115:GLY:N	2.63	0.51
1:A:102:ILE:HG23	1:A:103:ALA:N	2.25	0.51
1:A:249:MET:SD	1:A:249:MET:O	2.68	0.51
1:B:106:VAL:O	1:B:109:ILE:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASP:CG	1:B:221:SER:HB3	2.30	0.51
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:208:MET:HE2	1:B:233:ALA:HB1	1.92	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:111:MET:O	1:A:115:GLY:N	2.45	0.49
1:A:100:MET:HG2	1:A:158:TRP:CE2	2.47	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: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:238:VAL:HG22	1:A:241:TRP:CE3	2.46	0.48
1:B:208:MET:HE1	1:B:233:ALA:HB1	1.94	0.48
1:B:98:TRP:HA	1:B:101:MET:HE2	1.95	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:B:106:VAL:HG12	1:B:106:VAL:O	2.13	0.48
1:A:102:ILE:CG2	1:A:103:ALA:N	2.77	0.48
1:B:210:TYR:HA	1:B:265:ALA:HB2	1.96	0.48
1:B:106:VAL:C	1:B:109:ILE:HG12	2.33	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: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:B:231:ILE:HG23	1:B:234:LEU:HB3	1.97	0.47
1:A:173:LYS:O	1:A:177:ILE:HG13	2.15	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:173:LYS:HZ2	1:A:268:ASP:CG	2.18	0.47
1:A:234:LEU:O	1:A:238:VAL:HB	2.15	0.46
1:A:243:ASP:OD1	1:A:243:ASP:O	2.32	0.46
1:A:236:TRP:CD1	1:A:236:TRP:N	2.81	0.46
1:A:113:ILE:HD13	1:A:113:ILE:HG21	1.48	0.46
1:B:231:ILE:HG23	1:B:234:LEU:HD13	1.98	0.46
1:A:97:THR:O	1:A:101:MET:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:VAL:HG23	1:A:171:SER:HB3	1.98	0.46
1:A:220:GLN:C	1:A:222:GLY:N	2.68	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:226:GLN:CB	1:A:229:LEU:HD12	2.46	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:120:MET:O	1:A:121:LEU:C	2.54	0.46
1:A:242:PHE:O	1:A:244:LEU:N	2.49	0.45
1:A:100:MET:CB	1:A:158:TRP:CZ2	3.00	0.45
1:B:252:GLY:C	1:B:254:HIS:H	2.20	0.45
1:A:111:MET:O	1:A:115:GLY:CA	2.64	0.45
1:A:102:ILE:O	1:A:106:VAL:HG23	2.16	0.45
1:A:97:THR:O	1:A:101:MET:HG3	2.17	0.45
1:A:217:ARG:HH21	1:A:266:PHE:HE1	1.65	0.45
1:A:210:TYR:HA	1:A:265:ALA:HB2	1.99	0.45
1:B:231:ILE:HG12	1:B:231:ILE:H	1.43	0.44
1:B:235:ILE:O	1:B:239:ALA:CB	2.56	0.44
1:B:209:GLY:O	1:B:262:LEU:HD23	2.17	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: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:229:LEU:O	1:A:230:ILE:C	2.56	0.44
1:B:125:TRP:HE1	1:B:190:GLN:HG3	1.78	0.44
1:A:242:PHE:C	1:A:244:LEU:N	2.66	0.44
1:A:126:PRO:HD3	1:A:137:ARG:HB3	1.99	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:190:GLN:CD	1:A:191:LYS:N	2.72	0.43
1:A:158:TRP:O	1:A:162:GLY:N	2.52	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
1:A:96:VAL:HG21	1:A:171:SER:HB3	2.00	0.43
1:B:98:TRP:HA	1:B:101:MET:CE	2.48	0.43
1:A:271:ASN:ND2	1:B:191:LYS:HE3	2.33	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:MET:CE	1:B:233:ALA:CB	2.96	0.42
1:B:102:ILE:HG23	1:B:103:ALA:N	2.35	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:234:LEU:HD23	1:B:238:VAL:HG23	2.02	0.41
1:B:141:HIS:O	1:B:198:GLY:HA2	2.20	0.41
1:A:232:PHE:CD2	1:A:235:ILE:HD12	2.55	0.41
1:B:106:VAL:HA	1:B:109:ILE:HG13	1.91	0.41
1:A:249:MET:CG	1:A:249:MET:O	2.68	0.41
1:B:234:LEU:O	1:B:238:VAL:HG23	2.21	0.41
1:B:127:PHE:CE1	1:B:131:LEU:CD1	3.03	0.41
1:A:244:LEU:HD23	1:A:245:PHE:H	1.80	0.41
1:A:104:CYS:SG	1:A:200:LEU:HD22	2.61	0.41
1:A:162:GLY:O	1:A:163:GLY:C	2.58	0.41
1:B:94:GLY:HA3	1:B:166:GLU:CD	2.41	0.41
1:A:234:LEU:C	1:A:236:TRP:N	2.68	0.41
1:A:244:LEU:HD23	1:A:245:PHE:O	2.21	0.41
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.75	0.41
1:B:160:TYR:CE2	1:B:229:LEU:HD12	2.55	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:160:TYR:CE2	1:B:229:LEU:CD1	3.03	0.41
1:B:148:LEU:HD12	1:B:148:LEU:HA	1.82	0.41
1:A:236:TRP:HA	1:A:239:ALA:HB3	2.03	0.40
1:B:141:HIS:HA	1:B:144:MET:CE	2.51	0.40
1:A:206:ALA:HB2	1:A:257:GLY:O	2.20	0.40
1:B:141:HIS:HA	1:B:144:MET:HE2	2.03	0.40
1:B:223:ILE:CG2	1:B:223:ILE:O	2.68	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	A	180/182 (99%)	148 (82%)	24 (13%)	8 (4%)	3 4
1	B	169/182 (93%)	151 (89%)	13 (8%)	5 (3%)	5 8
All	All	349/364 (96%)	299 (86%)	37 (11%)	13 (4%)	4 5

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 (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	A	145/145 (100%)	130 (90%)	15 (10%)	9 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	138/145 (95%)	123 (89%)	15 (11%)	8 14
All	All	283/290 (98%)	253 (89%)	30 (11%)	8 15

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

Mol	Chain	Res	Type
1	A	121	LEU
1	A	126	PRO
1	A	130	THR
1	A	131	LEU
1	A	143	LEU
1	A	184	LEU
1	A	190	GLN
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	190	GLN
1	B	213	LEU
1	B	214	ARG
1	B	217	ARG
1	B	226	GLN
1	B	231	ILE
1	B	236	TRP
1	B	241	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN

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Mol	Chain	Res	Type
1	A	145	HIS
1	A	154	ASN
1	A	190	GLN
1	A	271	ASN
1	B	154	ASN
1	B	251	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	1.53	44 (24%)	1	0	30, 88, 134, 158	0
1	B	173/182 (95%)	1.67	57 (32%)	0	0	37, 98, 156, 162	0
All	All	355/364 (97%)	1.59	101 (28%)	1	0	30, 94, 149, 162	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ILE	16.5
1	B	229	LEU	10.9
1	A	232	PHE	8.7
1	B	232	PHE	8.7
1	A	222	GLY	7.7
1	B	98	TRP	7.4
1	B	227	ARG	6.6
1	B	225	LEU	6.2
1	A	139	PHE	6.2
1	A	270	LEU	6.1
1	A	196	TRP	6.1
1	A	220	GLN	6.0
1	A	169	LEU	5.8
1	A	200	LEU	5.8
1	A	217	ARG	5.7
1	B	236	TRP	5.4
1	A	98	TRP	5.3
1	A	271	ASN	5.0
1	B	159	TRP	4.7
1	A	247	MET	4.7
1	B	211	VAL	4.7
1	A	227	ARG	4.6
1	B	176	VAL	4.4
1	B	160	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	4.2
1	B	231	ILE	3.9
1	A	245	PHE	3.8
1	A	234	LEU	3.8
1	B	189	GLN	3.8
1	B	235	ILE	3.7
1	A	248	SER	3.7
1	A	168	ARG	3.6
1	B	217	ARG	3.6
1	A	219	PRO	3.6
1	B	230	ILE	3.5
1	B	153	PHE	3.5
1	B	205	TYR	3.4
1	A	243	ASP	3.4
1	B	239	ALA	3.3
1	A	127	PHE	3.3
1	B	127	PHE	3.2
1	B	152	LEU	3.2
1	B	240	GLY	3.2
1	B	169	LEU	3.2
1	A	192	PHE	3.2
1	B	154	ASN	3.1
1	B	226	GLN	3.1
1	B	107	VAL	3.1
1	A	229	LEU	3.1
1	B	187	TYR	3.1
1	B	191	LYS	3.0
1	A	149	MET	3.0
1	B	200	LEU	3.0
1	B	228	GLY	3.0
1	B	135	PHE	2.9
1	B	251	ASN	2.9
1	A	233	ALA	2.9
1	B	157	TRP	2.9
1	A	128	ASP	2.9
1	B	237	ILE	2.8
1	A	272	ALA	2.8
1	B	188	VAL	2.8
1	B	212	TRP	2.7
1	A	246	GLY	2.6
1	A	249	MET	2.6
1	A	130	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	150	HIS	2.6
1	B	255	ILE	2.6
1	A	242	PHE	2.6
1	B	122	TRP	2.6
1	A	224	TYR	2.6
1	B	210	TYR	2.6
1	B	265	ALA	2.6
1	B	131	LEU	2.5
1	A	167	LYS	2.5
1	B	95	PRO	2.5
1	B	241	TRP	2.5
1	B	91	GLU	2.5
1	B	156	LEU	2.5
1	A	250	ALA	2.4
1	A	228	GLY	2.4
1	B	196	TRP	2.4
1	B	266	PHE	2.4
1	B	158	TRP	2.4
1	B	234	LEU	2.3
1	B	133	PHE	2.3
1	B	114	LEU	2.3
1	A	221	SER	2.3
1	B	267	VAL	2.3
1	B	162	GLY	2.3
1	A	195	PRO	2.3
1	B	223	ILE	2.2
1	A	100	MET	2.2
1	B	207	LEU	2.2
1	A	266	PHE	2.2
1	B	155	LEU	2.2
1	A	218	ASP	2.2
1	A	206	ALA	2.1
1	A	197	PHE	2.0
1	A	152	LEU	2.0
1	B	151	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.