Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 03:51 AM EDT

PDB ID	:	2G98
Title	:	human gamma-D-crystallin
Authors	:	Kmoch, S.; Brynda, J.; Awsav, B.; Bezouska, K.; Novak, P.; Rezacova, P.
Deposited on	:	2006-03-06
Resolution	:	2.20 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:

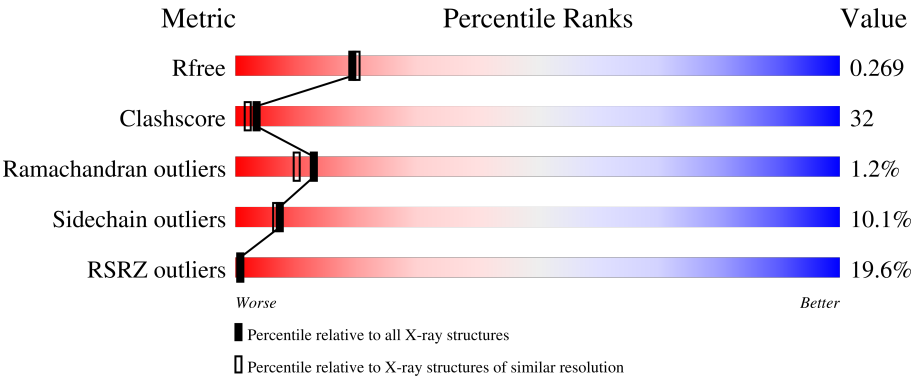
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	173	3% 66% 24% 7%
1	B	173	35% 48% 34% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2919 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 Gamma crystallin D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1395	867	257	261	10			
1	B	170	Total	C	N	O	S	0	0	0
			1372	859	250	253	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	SER	ARG	engineered mutation	UNP P07320
B	36	SER	ARG	engineered mutation	UNP P07320

- Molecule 2 is water.

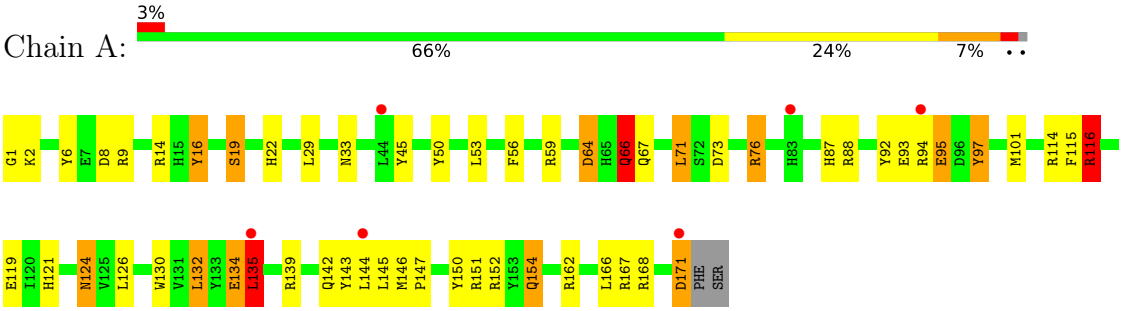
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		
2	B	65	Total	O	0	0
			65	65		

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.

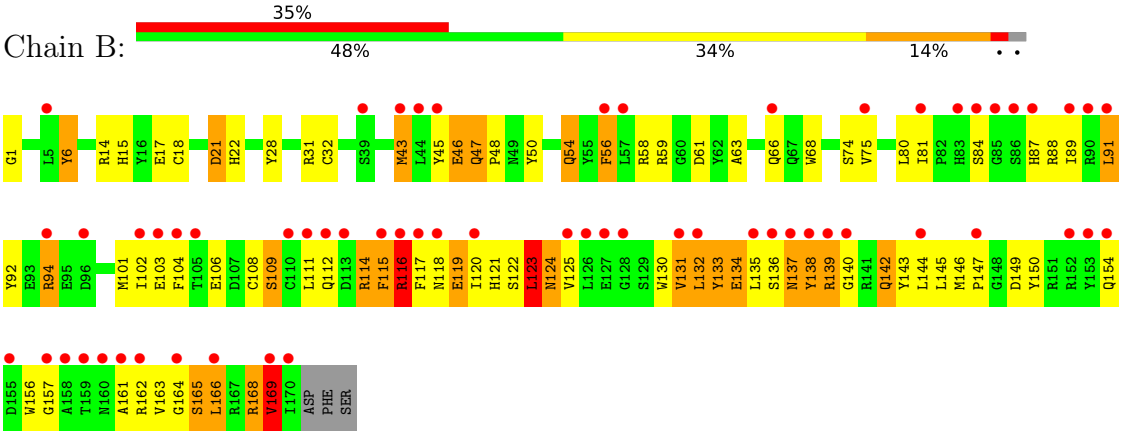
• Molecule 1: Gamma crystallin D

Chain A:



• Molecule 1: Gamma crystallin D

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.38Å 81.78Å 106.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.90 – 2.20 29.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.90-2.20) 91.2 (29.68-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.197 , 0.257 0.206 , 0.269	Depositor DCC
R_{free} test set	1153 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2919	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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, 0.333 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	1.71	17/1431 (1.2%)	1.44	17/1933 (0.9%)
1	B	1.90	25/1409 (1.8%)	1.46	15/1906 (0.8%)
All	All	1.81	42/2840 (1.5%)	1.45	32/3839 (0.8%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	VAL	CA-CB	11.99	1.79	1.54
1	B	108	CYS	CB-SG	10.07	1.99	1.82
1	B	54	GLN	CB-CG	9.94	1.79	1.52
1	A	76	ARG	CG-CD	-9.08	1.29	1.51
1	B	63	ALA	CA-CB	9.06	1.71	1.52
1	B	56	PHE	CA-CB	8.48	1.72	1.53
1	B	56	PHE	CG-CD2	8.04	1.50	1.38
1	B	18	CYS	CB-SG	-8.02	1.68	1.82
1	B	56	PHE	CE1-CZ	7.62	1.51	1.37
1	B	28	TYR	CD1-CE1	7.44	1.50	1.39
1	B	50	TYR	CE1-CZ	7.23	1.48	1.38
1	B	6	TYR	CE1-CZ	-6.63	1.29	1.38
1	B	131	VAL	CA-CB	6.55	1.68	1.54
1	A	95	GLU	CD-OE2	6.38	1.32	1.25
1	A	45	TYR	CE1-CZ	-6.30	1.30	1.38
1	B	58	ARG	CA-CB	6.18	1.67	1.53
1	A	143	TYR	CD1-CE1	6.03	1.48	1.39
1	A	8	ASP	C-O	6.00	1.34	1.23
1	A	151	ARG	CA-CB	5.99	1.67	1.53
1	B	134	GLU	CB-CG	-5.92	1.41	1.52
1	B	6	TYR	CD1-CE1	-5.90	1.30	1.39
1	B	43	MET	CG-SD	5.72	1.96	1.81
1	A	16	TYR	CE2-CZ	5.51	1.45	1.38
1	B	45	TYR	CZ-OH	5.47	1.47	1.37
1	B	56	PHE	CA-C	5.46	1.67	1.52
1	A	2	LYS	CE-NZ	5.40	1.62	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	LEU	C-O	-5.33	1.13	1.23
1	B	143	TYR	CG-CD1	-5.30	1.32	1.39
1	A	134	GLU	CD-OE1	-5.28	1.19	1.25
1	A	50	TYR	CG-CD1	-5.27	1.32	1.39
1	B	138	TYR	CD1-CE1	5.26	1.47	1.39
1	A	150	TYR	CD1-CE1	-5.25	1.31	1.39
1	A	66	GLN	CG-CD	5.24	1.63	1.51
1	B	68	TRP	C-O	-5.24	1.13	1.23
1	B	106	GLU	CA-CB	5.22	1.65	1.53
1	A	71	LEU	C-O	-5.20	1.13	1.23
1	B	132	LEU	C-O	-5.19	1.13	1.23
1	A	124	ASN	N-CA	-5.13	1.36	1.46
1	B	139	ARG	CB-CG	5.11	1.66	1.52
1	A	6	TYR	CD2-CE2	5.08	1.47	1.39
1	A	97	TYR	CA-CB	5.07	1.65	1.53
1	B	59	ARG	CA-CB	5.00	1.65	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	PHE	CB-CG-CD2	-11.15	112.99	120.80
1	B	14	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	A	171	ASP	CB-CG-OD1	10.05	127.34	118.30
1	A	76	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	76	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	A	73	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	162	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	114	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	145	LEU	CB-CG-CD1	-7.50	98.24	111.00
1	B	91	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	B	169	VAL	CA-CB-CG1	7.11	121.57	110.90
1	A	167	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	171	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	168	ARG	O-C-N	-6.82	111.79	122.70
1	B	91	LEU	CB-CG-CD2	6.75	122.47	111.00
1	A	29	LEU	CA-CB-CG	6.67	130.64	115.30
1	A	144	LEU	CB-CG-CD2	-6.26	100.35	111.00
1	B	56	PHE	CB-CG-CD1	6.18	125.13	120.80
1	A	168	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	56	PHE	N-CA-CB	-6.08	99.66	110.60
1	B	133	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	19	SER	CA-CB-OG	-5.76	95.66	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	B	123	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	135	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	14	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	143	TYR	N-CA-CB	-5.41	100.87	110.60
1	A	59	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	94	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	31	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	139	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	61	ASP	CB-CG-OD1	-5.06	113.75	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1395	0	1282	36	0
1	B	1372	0	1255	134	0
2	A	87	0	0	12	0
2	B	65	0	0	48	0
All	All	2919	0	2537	170	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 32.

All (170) 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:B:169:VAL:CA	1:B:169:VAL:CB	1.79	1.58
1:B:54:GLN:CB	1:B:54:GLN:CG	1.79	1.57
1:B:81:ILE:CD1	1:B:81:ILE:CG1	1.83	1.56
1:B:145:LEU:HD21	2:B:177:HOH:O	1.28	1.26
1:A:166:LEU:HB2	2:A:246:HOH:O	1.31	1.25
1:B:166:LEU:HD12	2:B:203:HOH:O	1.46	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HG13	2:B:211:HOH:O	1.52	1.09
1:B:134:GLU:HG3	1:B:135:LEU:HD13	1.38	1.03
1:B:22:HIS:HD2	2:B:197:HOH:O	1.41	1.01
1:B:135:LEU:HA	2:B:238:HOH:O	1.61	1.00
1:B:91:LEU:HB3	2:B:181:HOH:O	1.61	0.99
1:A:132:LEU:HD12	1:A:166:LEU:CD1	1.94	0.97
1:B:102:ILE:HG22	1:B:115:PHE:CE1	2.00	0.95
1:B:111:LEU:HA	2:B:236:HOH:O	1.65	0.95
1:B:132:LEU:HD11	1:B:163:VAL:HG11	1.47	0.95
1:B:124:ASN:CB	2:B:176:HOH:O	2.18	0.92
1:A:154:GLN:HE21	1:A:154:GLN:H	1.13	0.91
1:B:123:LEU:HB2	2:B:217:HOH:O	1.71	0.89
1:B:22:HIS:CD2	2:B:197:HOH:O	2.15	0.89
1:B:91:LEU:HD22	2:B:222:HOH:O	1.73	0.88
1:B:109:SER:CB	2:B:237:HOH:O	2.21	0.87
1:B:156:TRP:CE3	2:B:206:HOH:O	2.26	0.87
1:B:112:GLN:HG2	2:B:183:HOH:O	1.75	0.85
1:B:56:PHE:HB3	1:B:142:GLN:HE21	1.41	0.84
1:B:134:GLU:HG3	1:B:135:LEU:CD1	2.07	0.84
1:A:124:ASN:CB	2:A:178:HOH:O	2.26	0.83
1:A:53:LEU:CB	2:A:204:HOH:O	2.26	0.83
1:B:142:GLN:OE1	2:B:231:HOH:O	1.96	0.83
1:B:89:ILE:HG22	1:B:104:PHE:HB2	1.61	0.81
1:B:43:MET:HE1	1:B:56:PHE:HB2	1.65	0.79
1:B:102:ILE:CG2	1:B:115:PHE:CE1	2.66	0.78
1:B:169:VAL:CA	1:B:169:VAL:HB	2.10	0.77
1:A:166:LEU:HD22	2:A:246:HOH:O	1.84	0.77
1:A:132:LEU:CD1	1:A:166:LEU:CD1	2.65	0.75
1:B:109:SER:HB3	2:B:200:HOH:O	1.85	0.75
1:B:165:SER:N	2:B:224:HOH:O	2.19	0.74
1:A:154:GLN:H	1:A:154:GLN:NE2	1.84	0.74
1:B:56:PHE:CD1	1:B:131:VAL:HG21	2.22	0.74
1:A:132:LEU:CD1	1:A:166:LEU:HD11	2.16	0.74
1:A:97:TYR:CB	2:A:243:HOH:O	2.36	0.73
1:B:162:ARG:HB3	2:B:193:HOH:O	1.87	0.73
1:B:56:PHE:HB3	1:B:142:GLN:NE2	2.03	0.72
1:B:102:ILE:CD1	1:B:104:PHE:CZ	2.73	0.72
1:B:146:MET:HB3	1:B:147:PRO:HD2	1.72	0.71
1:B:133:TYR:HB3	1:B:139:ARG:O	1.91	0.71
1:B:43:MET:HE1	1:B:56:PHE:CB	2.21	0.71
1:B:135:LEU:CA	2:B:238:HOH:O	2.26	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:H	1:A:142:GLN:HE22	1.39	0.71
1:B:109:SER:HB2	2:B:237:HOH:O	1.88	0.70
1:B:1:GLY:N	2:B:207:HOH:O	2.24	0.69
1:B:140:GLY:HA2	2:B:194:HOH:O	1.91	0.69
1:B:102:ILE:HD11	1:B:104:PHE:CZ	2.28	0.69
1:A:53:LEU:CB	2:A:205:HOH:O	2.42	0.68
1:B:92:TYR:CE2	1:B:101:MET:HG3	2.30	0.67
1:B:91:LEU:C	2:B:181:HOH:O	2.32	0.67
1:B:135:LEU:C	2:B:224:HOH:O	2.33	0.67
1:B:134:GLU:CG	1:B:135:LEU:HD13	2.20	0.67
1:A:115:PHE:O	1:A:116:ARG:CB	2.42	0.66
1:B:135:LEU:CD1	2:B:232:HOH:O	2.43	0.66
1:B:54:GLN:HB2	1:B:142:GLN:O	1.96	0.66
1:B:111:LEU:CA	2:B:236:HOH:O	2.29	0.66
1:B:120:ILE:HD12	2:B:181:HOH:O	1.95	0.65
1:B:135:LEU:O	2:B:224:HOH:O	2.13	0.64
1:A:97:TYR:CB	2:A:253:HOH:O	2.45	0.64
1:B:102:ILE:HG21	1:B:115:PHE:CD1	2.33	0.64
1:B:168:ARG:O	1:B:169:VAL:CB	2.46	0.63
1:B:54:GLN:CG	1:B:54:GLN:CA	2.77	0.62
1:A:64:ASP:HB2	1:A:66:GLN:HE21	1.65	0.62
1:A:139:ARG:HD2	2:A:250:HOH:O	1.98	0.62
1:A:93:GLU:OE2	1:A:94:ARG:NH1	2.33	0.61
1:B:131:VAL:HG23	1:B:169:VAL:HG12	1.83	0.61
1:A:92:TYR:CE2	1:A:101:MET:HG3	2.35	0.60
1:B:43:MET:CE	1:B:56:PHE:HB2	2.31	0.60
1:A:166:LEU:CD2	2:A:246:HOH:O	2.47	0.59
1:B:91:LEU:HD13	2:B:211:HOH:O	2.02	0.59
1:A:132:LEU:HD13	1:A:166:LEU:HD11	1.83	0.58
1:A:132:LEU:HD12	1:A:166:LEU:HD13	1.85	0.58
1:B:102:ILE:HD13	1:B:104:PHE:CZ	2.38	0.57
1:B:102:ILE:CG2	1:B:115:PHE:CD1	2.88	0.56
1:A:115:PHE:O	1:A:116:ARG:HB2	2.04	0.56
1:B:92:TYR:CE2	1:B:101:MET:CG	2.89	0.56
1:B:56:PHE:H	1:B:142:GLN:NE2	2.04	0.55
1:B:109:SER:O	1:B:137:ASN:N	2.23	0.55
1:B:138:TYR:CD1	1:B:165:SER:HB2	2.41	0.55
1:B:43:MET:HE1	1:B:56:PHE:N	2.21	0.55
1:A:87:HIS:HB3	1:A:130:TRP:CZ2	2.42	0.55
1:B:56:PHE:CB	1:B:142:GLN:HE21	2.15	0.55
1:B:87:HIS:HB3	1:B:130:TRP:CZ2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD12	2:B:236:HOH:O	2.06	0.54
1:B:84:SER:HB2	1:B:87:HIS:CE1	2.43	0.54
1:B:135:LEU:C	2:B:238:HOH:O	2.45	0.54
1:B:91:LEU:CA	2:B:181:HOH:O	2.56	0.53
1:B:94:ARG:CG	1:B:94:ARG:HH11	2.20	0.53
1:B:132:LEU:HD11	1:B:163:VAL:CG1	2.29	0.53
1:B:88:ARG:CB	2:B:204:HOH:O	2.55	0.53
1:B:149:ASP:C	1:B:150:TYR:CD1	2.82	0.53
1:B:134:GLU:HG2	1:B:140:GLY:HA3	1.91	0.53
1:B:131:VAL:HG23	1:B:169:VAL:CG1	2.39	0.53
1:B:81:ILE:CG2	1:B:144:LEU:HD11	2.40	0.52
1:B:89:ILE:O	1:B:89:ILE:CG2	2.56	0.52
1:B:54:GLN:CB	1:B:54:GLN:CD	2.74	0.52
1:B:104:PHE:HA	2:B:195:HOH:O	2.10	0.52
1:A:134:GLU:HG2	1:A:135:LEU:HD13	1.93	0.51
1:B:91:LEU:CD2	2:B:222:HOH:O	2.41	0.51
1:B:89:ILE:O	1:B:89:ILE:HG23	2.09	0.51
1:B:81:ILE:CD1	1:B:81:ILE:CB	2.82	0.50
1:B:103:GLU:HG2	2:B:226:HOH:O	2.11	0.50
1:B:81:ILE:HG23	1:B:144:LEU:HD11	1.94	0.50
1:B:137:ASN:N	1:B:137:ASN:ND2	2.59	0.50
1:B:140:GLY:C	2:B:185:HOH:O	2.50	0.50
1:B:135:LEU:HD11	2:B:232:HOH:O	2.11	0.50
1:B:169:VAL:CA	1:B:169:VAL:CG2	2.82	0.49
1:B:119:GLU:HA	1:B:161:ALA:O	2.12	0.49
1:B:164:GLY:HA3	2:B:238:HOH:O	2.13	0.49
1:B:43:MET:SD	1:B:56:PHE:HA	2.54	0.48
1:B:102:ILE:HG22	1:B:115:PHE:CZ	2.47	0.48
1:B:116:ARG:O	1:B:117:PHE:CG	2.67	0.48
1:B:135:LEU:O	1:B:165:SER:OG	2.32	0.48
1:A:88:ARG:HG2	1:A:126:LEU:HD12	1.97	0.47
1:B:123:LEU:O	1:B:124:ASN:CB	2.62	0.47
1:B:133:TYR:CD1	1:B:133:TYR:N	2.82	0.47
1:B:43:MET:CE	1:B:56:PHE:N	2.78	0.47
1:B:43:MET:SD	1:B:56:PHE:HB2	2.54	0.47
1:B:56:PHE:C	1:B:56:PHE:CD2	2.87	0.47
1:B:119:GLU:HB3	1:B:161:ALA:CB	2.45	0.47
1:B:46:GLU:HG2	1:B:47:GLN:HG2	1.96	0.47
1:B:102:ILE:CD1	1:B:104:PHE:CE1	2.98	0.46
1:B:89:ILE:CG2	1:B:104:PHE:HB2	2.38	0.46
1:B:161:ALA:O	1:B:163:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HD12	2:B:232:HOH:O	2.11	0.46
1:B:32:CYS:HB3	1:B:75:VAL:HG23	1.98	0.45
1:B:81:ILE:HG12	1:B:144:LEU:CD1	2.46	0.45
1:B:149:ASP:C	1:B:150:TYR:HD1	2.19	0.45
1:B:94:ARG:HH11	1:B:94:ARG:HG3	1.81	0.45
1:B:125:VAL:HG21	1:B:146:MET:O	2.16	0.45
1:B:132:LEU:CD1	1:B:163:VAL:HG11	2.31	0.45
1:B:137:ASN:N	1:B:137:ASN:HD22	2.15	0.45
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.81	0.45
1:B:124:ASN:C	2:B:217:HOH:O	2.54	0.45
1:A:56:PHE:H	1:A:142:GLN:NE2	2.12	0.45
1:A:92:TYR:CE2	1:A:101:MET:CG	3.00	0.44
1:B:43:MET:SD	1:B:56:PHE:CA	3.06	0.44
1:B:136:SER:N	2:B:238:HOH:O	2.50	0.44
1:A:139:ARG:NH1	2:A:216:HOH:O	2.50	0.43
1:A:146:MET:HB3	1:A:147:PRO:HD2	2.00	0.43
1:B:125:VAL:HB	1:B:147:PRO:HA	2.00	0.43
1:B:132:LEU:HD13	2:B:222:HOH:O	2.18	0.43
1:B:169:VAL:CB	1:B:169:VAL:C	2.78	0.43
1:B:149:ASP:CB	2:B:188:HOH:O	2.67	0.42
1:B:157:GLY:C	2:B:189:HOH:O	2.57	0.42
1:A:166:LEU:CG	2:A:246:HOH:O	2.54	0.42
1:A:33:ASN:O	1:A:64:ASP:HA	2.20	0.42
1:B:102:ILE:HG21	1:B:102:ILE:HD13	1.78	0.42
1:B:1:GLY:H1	1:B:80:LEU:HD21	1.85	0.42
1:B:132:LEU:HG	1:B:163:VAL:HG13	2.02	0.42
1:A:1:GLY:N	2:A:207:HOH:O	2.52	0.42
1:B:43:MET:HE1	1:B:56:PHE:CA	2.50	0.41
1:B:121:HIS:O	1:B:122:SER:HB2	2.20	0.41
1:A:119:GLU:OE1	1:A:121:HIS:CE1	2.74	0.41
1:B:156:TRP:HB2	2:B:177:HOH:O	2.20	0.41
1:B:114:ARG:N	2:B:199:HOH:O	2.52	0.41
1:B:21:ASP:OD1	1:B:21:ASP:N	2.52	0.41
1:B:111:LEU:C	2:B:236:HOH:O	2.54	0.41
1:A:16:TYR:OH	1:A:22:HIS:HE1	2.04	0.41
1:B:6:TYR:CD2	1:B:15:HIS:HB3	2.56	0.41
1:B:132:LEU:CD1	1:B:163:VAL:CG1	2.97	0.41
1:B:47:GLN:HB3	1:B:48:PRO:CD	2.51	0.41
1:B:102:ILE:HD13	1:B:104:PHE:CE1	2.56	0.40
1:B:118:ASN:C	1:B:119:GLU:HG2	2.38	0.40
1:A:132:LEU:HD12	1:A:166:LEU:HD12	1.91	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	169/173 (98%)	164 (97%)	4 (2%)	1 (1%)	25 26
1	B	168/173 (97%)	144 (86%)	21 (12%)	3 (2%)	8 5
All	All	337/346 (97%)	308 (91%)	25 (7%)	4 (1%)	13 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	B	116	ARG
1	B	124	ASN
1	B	169	VAL

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	146/155 (94%)	134 (92%)	12 (8%)	11 11
1	B	141/155 (91%)	124 (88%)	17 (12%)	5 4
All	All	287/310 (93%)	258 (90%)	29 (10%)	7 7

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	19	SER
1	A	66	GLN
1	A	67	GLN
1	A	71	LEU
1	A	76	ARG
1	A	95	GLU
1	A	116	ARG
1	A	135	LEU
1	A	152	ARG
1	A	154	GLN
1	A	171	ASP
1	B	17	GLU
1	B	21	ASP
1	B	46	GLU
1	B	47	GLN
1	B	66	GLN
1	B	74	SER
1	B	109	SER
1	B	114	ARG
1	B	115	PHE
1	B	116	ARG
1	B	119	GLU
1	B	123	LEU
1	B	137	ASN
1	B	142	GLN
1	B	154	GLN
1	B	165	SER
1	B	166	LEU

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

Mol	Chain	Res	Type
1	A	22	HIS
1	A	66	GLN
1	A	121	HIS
1	A	142	GLN
1	A	154	GLN
1	B	83	HIS
1	B	142	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

There are no monosaccharides 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	171/173 (98%)	0.44	6 (3%) 44 42	46, 56, 65, 74	0
1	B	170/173 (98%)	1.57	61 (35%) 0 0	51, 62, 70, 75	0
All	All	341/346 (98%)	1.01	67 (19%) 1 1	46, 60, 69, 75	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	HIS	7.4
1	B	116	ARG	6.2
1	B	136	SER	6.1
1	B	118	ASN	5.9
1	B	158	ALA	5.8
1	B	86	SER	5.4
1	B	111	LEU	5.1
1	B	120	ILE	5.1
1	B	131	VAL	4.9
1	B	128	GLY	4.6
1	B	85	GLY	4.3
1	B	137	ASN	4.3
1	B	153	TYR	4.2
1	B	161	ALA	3.9
1	B	144	LEU	3.7
1	B	96	ASP	3.7
1	B	43	MET	3.5
1	B	160	ASN	3.5
1	B	56	PHE	3.4
1	B	135	LEU	3.4
1	B	81	ILE	3.3
1	B	147	PRO	3.2
1	B	126	LEU	3.2
1	B	164	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	SER	3.2
1	B	157	GLY	3.1
1	B	132	LEU	3.0
1	B	94	ARG	3.0
1	B	44	LEU	3.0
1	B	87	HIS	3.0
1	B	166	LEU	2.9
1	B	105	THR	2.9
1	B	104	PHE	2.7
1	B	159	THR	2.7
1	B	127	GLU	2.6
1	B	170	ILE	2.6
1	B	152	ARG	2.5
1	B	117	PHE	2.5
1	B	90	ARG	2.5
1	A	144	LEU	2.5
1	B	138	TYR	2.5
1	B	45	TYR	2.5
1	B	103	GLU	2.5
1	B	110	CYS	2.5
1	A	135	LEU	2.5
1	B	125	VAL	2.4
1	B	5	LEU	2.4
1	B	39	SER	2.4
1	B	91	LEU	2.4
1	A	171	ASP	2.3
1	B	155	ASP	2.2
1	B	115	PHE	2.2
1	B	57	LEU	2.2
1	B	169	VAL	2.1
1	A	44	LEU	2.1
1	B	102	ILE	2.1
1	B	139	ARG	2.1
1	B	140	GLY	2.1
1	A	94	ARG	2.1
1	B	89	ILE	2.1
1	B	154	GLN	2.1
1	B	112	GLN	2.1
1	B	162	ARG	2.1
1	A	83	HIS	2.0
1	B	113	ASP	2.0
1	B	75	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	66	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 monosaccharides 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.