Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:01 am BST

PDB ID	:	1WR6
Title	:	Crystal structure of GGA3 GAT domain in complex with ubiquitin
Authors	:	Kawasaki, M.; Shiba, T.; Shiba, Y.; Yamaguchi, Y.; Matsugaki, N.; Igarashi, N.; Suzuki, M.; Kato, R.; Kato, K.; Nakayama, K.; Wakatsuki, S.
Deposited on	:	2004-10-12
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 following versions of software and data (see references ⓘ) were used in the production of this report:

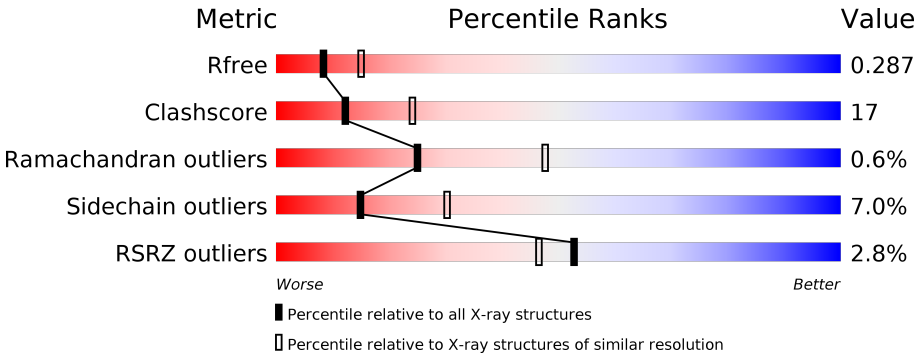
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	111	9% 53% 28% 19%
1	B	111	55% 20% 5% • 19%
1	C	111	% 58% 21% • 19%
1	D	111	5% 52% 22% 5% 21%
2	E	76	57% 33% 5% 5%
2	F	76	3% 45% 47% • •

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Mol	Chain	Length	Quality of chain
2	G	76	
2	H	76	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5327 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 ADP-ribosylation factor binding protein GGA3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	Se	0	0	0
			728	442	129	154	1	2			
1	B	90	Total	C	N	O	S	Se	0	0	0
			721	438	126	154	1	2			
1	C	90	Total	C	N	O	S	Se	0	0	0
			728	442	129	154	1	2			
1	D	88	Total	C	N	O	S	Se	0	0	0
			709	432	123	151	1	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
A	248	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
B	231	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
B	248	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
C	231	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
C	248	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
D	231	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52
D	248	MSE	MET	MODIFIED RESIDUE	UNP Q9NZ52

- Molecule 2 is a protein called ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	72	Total	C	N	O	S	0	0	0
			574	362	98	113	1			
2	F	73	Total	C	N	O	S	0	0	0
			582	368	99	114	1			
2	G	72	Total	C	N	O	S	0	0	0
			574	362	98	113	1			
2	H	74	Total	C	N	O	S	0	0	0
			593	374	103	115	1			

- Molecule 3 is water.

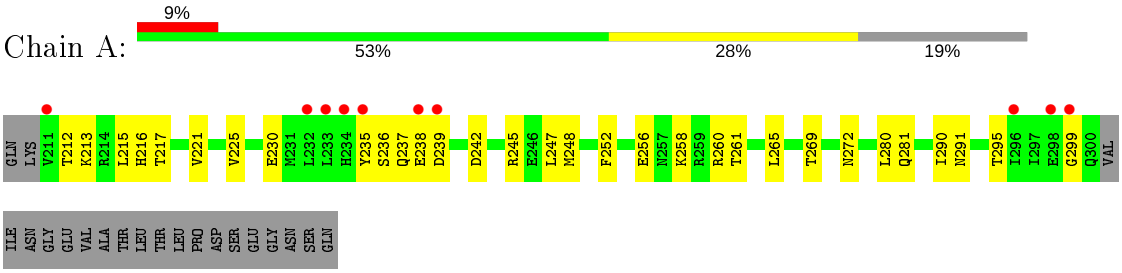
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	20	Total O 20 20	0	0
3	C	19	Total O 19 19	0	0
3	D	21	Total O 21 21	0	0
3	E	7	Total O 7 7	0	0
3	F	8	Total O 8 8	0	0
3	G	20	Total O 20 20	0	0
3	H	14	Total O 14 14	0	0

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 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.

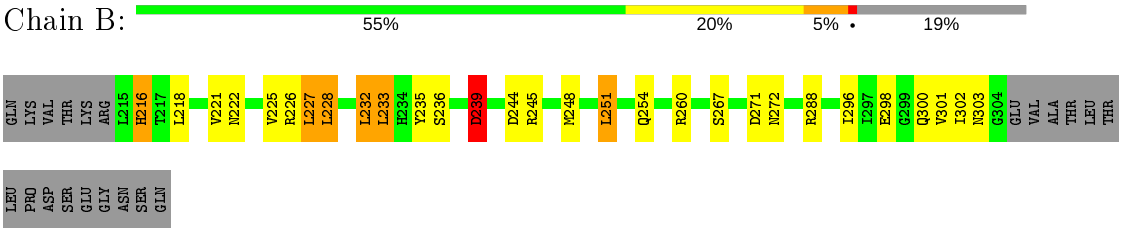
- Molecule 1: ADP-ribosylation factor binding protein GGA3

Chain A:



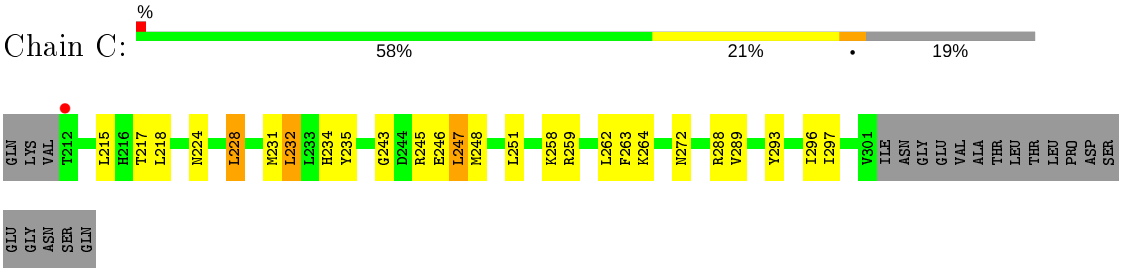
- Molecule 1: ADP-ribosylation factor binding protein GGA3

Chain B:



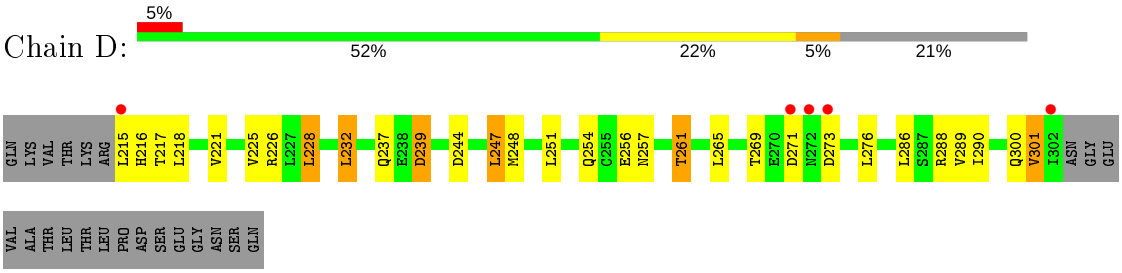
- Molecule 1: ADP-ribosylation factor binding protein GGA3

Chain C:



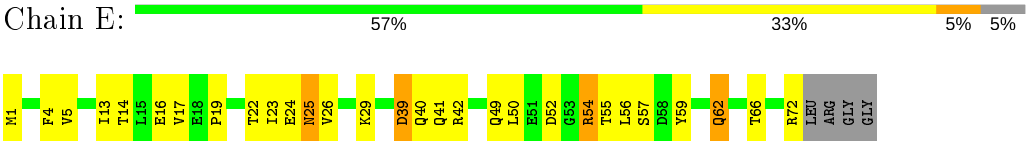
- Molecule 1: ADP-ribosylation factor binding protein GGA3

Chain D:



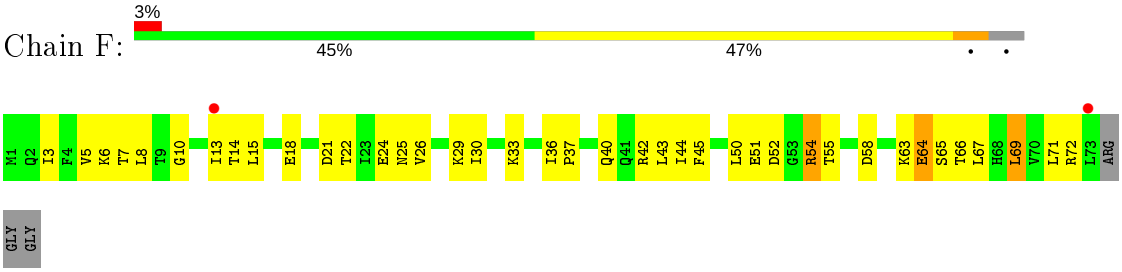
• Molecule 2: ubiquitin

Chain E:



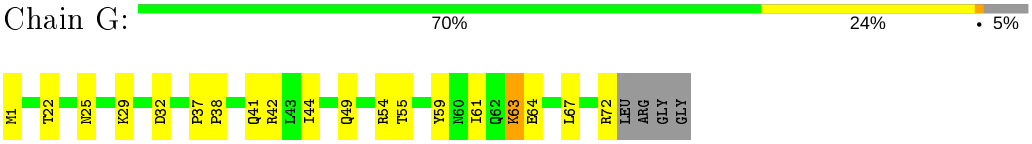
• Molecule 2: ubiquitin

Chain F:



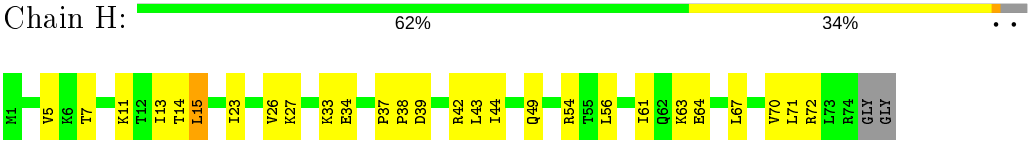
• Molecule 2: ubiquitin

Chain G:



• Molecule 2: ubiquitin

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.03Å 113.63Å 114.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 46.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (40.00-2.60) 94.5 (46.03-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.290 0.218 , 0.287	Depositor DCC
R_{free} test set	1105 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	0.35	0/731	0.51	0/978
1	B	0.42	0/724	0.55	0/970
1	C	0.41	0/731	0.58	0/978
1	D	0.41	0/712	0.62	0/954
2	E	0.35	0/580	0.54	0/781
2	F	0.34	0/588	0.54	0/792
2	G	0.39	0/580	0.66	0/781
2	H	0.43	0/599	0.71	1/806 (0.1%)
All	All	0.39	0/5245	0.59	1/7040 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	15	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	728	0	709	26	0
1	B	721	0	696	25	0
1	C	728	0	709	24	0
1	D	709	0	687	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	574	0	599	22	0
2	F	582	0	610	45	0
2	G	574	0	599	14	0
2	H	593	0	623	17	0
3	A	9	0	0	0	0
3	B	20	0	0	1	0
3	C	19	0	0	0	0
3	D	21	0	0	1	0
3	E	7	0	0	0	0
3	F	8	0	0	0	0
3	G	20	0	0	1	0
3	H	14	0	0	0	0
All	All	5327	0	5232	177	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 17.

All (177) 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)
2:F:22:THR:H	2:F:25:ASN:HD22	1.03	0.97
2:F:71:LEU:HD22	2:F:71:LEU:H	1.43	0.81
1:B:233:LEU:HD22	1:C:218:LEU:HG	1.61	0.80
1:A:247:LEU:HD13	2:E:42:ARG:HG2	1.66	0.77
2:E:24:GLU:HB2	2:E:52:ASP:HB3	1.65	0.77
1:A:212:THR:HG22	1:A:213:LYS:H	1.51	0.76
2:F:24:GLU:HG2	2:F:52:ASP:HB3	1.67	0.75
2:F:36:ILE:HD12	2:F:37:PRO:HD2	1.69	0.75
2:F:5:VAL:HG23	2:F:13:ILE:HG13	1.68	0.74
1:D:228:LEU:HD22	1:D:232:LEU:HD22	1.69	0.73
2:F:63:LYS:HB3	2:F:63:LYS:NZ	2.03	0.72
2:E:23:ILE:HB	2:E:52:ASP:HA	1.70	0.72
1:D:221:VAL:O	1:D:225:VAL:HG23	1.90	0.71
2:F:44:ILE:HD12	2:F:44:ILE:N	2.07	0.70
1:A:272:ASN:HD21	1:B:300:GLN:HE22	1.38	0.70
2:F:25:ASN:O	2:F:29:LYS:HG3	1.91	0.69
2:H:61:ILE:HD13	2:H:67:LEU:HD21	1.75	0.69
1:C:247:LEU:HG	2:G:49:GLN:HE21	1.59	0.67
2:F:36:ILE:HD11	2:F:40:GLN:HG3	1.76	0.67
1:C:231:MSE:HE1	1:C:251:LEU:HD23	1.76	0.67
2:E:22:THR:HG22	2:E:55:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:ILE:HD13	2:G:67:LEU:HD21	1.76	0.67
1:A:252:PHE:CE1	1:A:290:ILE:HG23	2.30	0.67
1:A:215:LEU:HD12	1:A:265:LEU:HD21	1.75	0.66
2:F:22:THR:N	2:F:25:ASN:HD22	1.86	0.66
1:C:231:MSE:HE1	1:C:251:LEU:CD2	2.26	0.65
2:F:22:THR:H	2:F:25:ASN:ND2	1.87	0.65
1:B:236:SER:OG	1:B:239:ASP:HB2	1.97	0.64
1:D:226:ARG:HG2	3:D:10:HOH:O	1.98	0.64
1:D:254:GLN:HA	1:D:254:GLN:HE21	1.63	0.64
2:F:5:VAL:HB	2:F:69:LEU:HD11	1.81	0.63
2:G:22:THR:HA	2:G:55:THR:HA	1.79	0.63
2:G:42:ARG:HH21	2:G:72:ARG:HG2	1.63	0.62
2:F:14:THR:C	2:F:15:LEU:HD12	2.20	0.62
1:B:235:TYR:HD2	1:B:248:MSE:HE1	1.65	0.61
2:F:5:VAL:CG2	2:F:13:ILE:HG13	2.29	0.61
2:H:7:THR:OG1	2:H:11:LYS:HB3	2.00	0.61
2:G:25:ASN:ND2	2:G:29:LYS:HE2	2.15	0.61
2:E:62:GLN:HA	2:E:62:GLN:HE21	1.65	0.61
1:A:213:LYS:CE	1:A:261:THR:HG22	2.31	0.61
1:A:272:ASN:ND2	1:B:300:GLN:HE22	1.99	0.61
2:F:14:THR:O	2:F:15:LEU:HD12	1.99	0.60
2:E:4:PHE:HD2	2:E:14:THR:HG22	1.66	0.60
1:D:288:ARG:HH11	1:D:288:ARG:HG2	1.67	0.60
2:E:25:ASN:O	2:E:29:LYS:HG3	2.01	0.60
2:F:63:LYS:HB3	2:F:63:LYS:HZ2	1.65	0.60
2:F:40:GLN:O	2:F:71:LEU:HA	2.01	0.60
2:H:14:THR:O	2:H:33:LYS:HE3	2.01	0.60
1:A:269:THR:O	1:B:260:ARG:HD3	2.01	0.59
1:B:228:LEU:HD22	1:B:232:LEU:HD22	1.84	0.59
1:B:288:ARG:NH2	1:C:264:LYS:HD2	2.17	0.59
2:E:54:ARG:HG3	2:E:59:TYR:OH	2.03	0.58
2:F:5:VAL:HB	2:F:69:LEU:CD1	2.33	0.58
1:A:291:ASN:O	1:A:295:THR:HG22	2.04	0.57
1:A:213:LYS:HE3	1:A:261:THR:HG22	1.85	0.57
1:D:254:GLN:HA	1:D:254:GLN:NE2	2.19	0.57
2:H:26:VAL:HG21	2:H:56:LEU:HD21	1.87	0.56
2:F:71:LEU:HD22	2:F:71:LEU:N	2.17	0.56
1:B:301:VAL:O	1:B:301:VAL:HG23	2.05	0.56
2:F:71:LEU:CD2	2:F:71:LEU:H	2.14	0.55
1:C:234:HIS:HD2	3:G:81:HOH:O	1.90	0.55
1:B:222:ASN:O	1:B:226:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:LEU:HD22	1:C:232:LEU:HD22	1.89	0.54
2:F:51:GLU:CB	2:F:54:ARG:HH11	2.20	0.54
2:F:33:LYS:O	2:F:33:LYS:HG2	2.07	0.54
2:F:26:VAL:O	2:F:30:ILE:HG13	2.07	0.53
1:C:247:LEU:HD13	2:G:44:ILE:HD11	1.89	0.53
1:C:224:ASN:HD22	1:C:258:LYS:HD2	1.73	0.53
2:H:42:ARG:HH21	2:H:72:ARG:HA	1.72	0.53
2:E:4:PHE:CD2	2:E:14:THR:HG22	2.44	0.53
2:H:23:ILE:HG12	2:H:54:ARG:O	2.09	0.52
2:H:63:LYS:O	2:H:64:GLU:HB2	2.10	0.52
1:B:271:ASP:O	1:B:272:ASN:HB2	2.08	0.52
2:F:43:LEU:HD23	2:F:69:LEU:HB3	1.91	0.52
2:F:5:VAL:HG12	2:F:67:LEU:HB2	1.91	0.52
2:E:62:GLN:CA	2:E:62:GLN:HE21	2.23	0.52
1:C:293:TYR:CE1	1:C:297:ILE:HG13	2.44	0.51
2:F:6:LYS:HD2	2:F:10:GLY:HA2	1.92	0.51
1:A:256:GLU:HG2	1:B:271:ASP:OD2	2.11	0.51
1:A:252:PHE:HE1	1:A:290:ILE:HG23	1.76	0.51
1:D:254:GLN:CA	1:D:254:GLN:HE21	2.22	0.51
2:E:5:VAL:HB	2:E:13:ILE:HG13	1.91	0.51
2:G:54:ARG:HB2	2:G:59:TYR:CE1	2.46	0.50
2:F:63:LYS:HG2	2:F:64:GLU:N	2.27	0.50
1:C:245:ARG:HA	1:C:248:MSE:HE3	1.93	0.50
2:F:45:PHE:HB3	2:F:50:LEU:HD21	1.93	0.50
2:G:54:ARG:HB2	2:G:59:TYR:HE1	1.76	0.50
1:A:245:ARG:HA	1:A:248:MSE:HE3	1.94	0.50
2:F:69:LEU:N	2:F:69:LEU:HD13	2.26	0.50
1:D:301:VAL:O	1:D:301:VAL:HG13	2.12	0.49
2:H:23:ILE:HG22	2:H:27:LYS:HE3	1.94	0.49
1:A:216:HIS:CD2	1:A:258:LYS:HG2	2.47	0.49
2:E:49:GLN:HG2	2:E:50:LEU:N	2.28	0.49
1:B:296:ILE:HD13	1:C:217:THR:CG2	2.43	0.49
1:A:221:VAL:O	1:A:225:VAL:HG23	2.12	0.49
2:F:63:LYS:HG2	2:F:64:GLU:OE1	2.13	0.48
2:F:36:ILE:HD12	2:F:37:PRO:CD	2.40	0.48
1:A:215:LEU:HD23	1:A:216:HIS:N	2.29	0.48
2:G:29:LYS:O	2:G:32:ASP:HB2	2.14	0.48
2:F:5:VAL:HA	2:F:67:LEU:O	2.14	0.48
1:A:260:ARG:HG2	1:B:267:SER:O	2.13	0.48
2:F:55:THR:O	2:F:58:ASP:HB2	2.14	0.48
1:B:228:LEU:O	1:B:232:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ASN:O	1:D:261:THR:HG23	2.14	0.47
1:C:272:ASN:HB2	2:F:65:SER:HA	1.96	0.47
2:H:43:LEU:O	2:H:49:GLN:HA	2.13	0.47
1:A:238:GLU:H	1:A:238:GLU:CD	2.17	0.47
1:B:221:VAL:O	1:B:225:VAL:HG23	2.13	0.47
1:D:269:THR:HG21	1:D:276:LEU:HB2	1.96	0.47
1:C:243:GLY:O	1:C:246:GLU:HG2	2.14	0.47
1:C:247:LEU:O	1:C:251:LEU:HD23	2.15	0.47
1:C:235:TYR:CD1	1:C:248:MSE:HE1	2.49	0.47
2:E:1:MET:HG2	2:E:17:VAL:O	2.14	0.47
2:F:42:ARG:O	2:F:69:LEU:HA	2.14	0.47
2:F:6:LYS:N	2:F:67:LEU:O	2.45	0.47
1:C:247:LEU:HD22	1:C:251:LEU:CD2	2.45	0.47
1:D:288:ARG:NH1	1:D:288:ARG:HG2	2.30	0.47
1:A:245:ARG:HG3	1:A:245:ARG:HH11	1.80	0.46
1:B:222:ASN:HD21	1:B:226:ARG:HD2	1.81	0.46
2:F:18:GLU:HB2	2:F:21:ASP:OD2	2.16	0.46
2:E:39:ASP:N	2:E:39:ASP:OD2	2.48	0.46
1:C:228:LEU:HD13	1:C:289:VAL:HG22	1.98	0.46
2:F:40:GLN:HA	2:F:72:ARG:HB3	1.98	0.46
1:B:298:GLU:HG2	3:B:116:HOH:O	2.15	0.46
1:D:247:LEU:HD11	2:H:44:ILE:HD11	1.98	0.46
2:H:5:VAL:HB	2:H:13:ILE:CG1	2.46	0.46
2:E:41:GLN:O	2:E:42:ARG:HD3	2.15	0.45
1:D:239:ASP:OD2	1:D:239:ASP:N	2.50	0.45
2:G:41:GLN:O	2:G:42:ARG:HG3	2.17	0.45
1:C:247:LEU:CD1	2:G:44:ILE:HD11	2.46	0.45
1:A:235:TYR:CD2	1:A:248:MSE:HE1	2.51	0.45
1:C:215:LEU:HD12	1:C:215:LEU:C	2.37	0.45
1:D:216:HIS:C	1:D:218:LEU:H	2.20	0.45
2:F:42:ARG:NH2	2:F:72:ARG:HA	2.31	0.45
1:A:217:THR:O	1:A:221:VAL:HG23	2.17	0.45
1:B:235:TYR:OH	1:B:245:ARG:NH1	2.50	0.45
1:D:256:GLU:HG2	1:D:290:ILE:HD13	1.99	0.45
1:D:300:GLN:O	1:D:301:VAL:C	2.56	0.45
1:A:272:ASN:HD21	1:B:300:GLN:NE2	2.11	0.45
1:B:216:HIS:C	1:B:218:LEU:H	2.19	0.45
2:H:44:ILE:N	2:H:44:ILE:HD12	2.32	0.45
1:C:247:LEU:HD12	2:G:49:GLN:HG3	2.00	0.44
1:B:227:LEU:HD13	1:B:251:LEU:HD21	2.00	0.44
1:B:244:ASP:HB3	1:B:248:MSE:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:GLN:HA	2:E:72:ARG:CD	2.47	0.44
2:E:54:ARG:HB2	2:E:59:TYR:CE1	2.52	0.44
2:H:37:PRO:HA	2:H:38:PRO:HD3	1.94	0.44
2:H:42:ARG:HB2	2:H:70:VAL:O	2.18	0.43
1:A:213:LYS:HE2	1:A:261:THR:HG22	1.99	0.43
2:E:4:PHE:O	2:E:66:THR:HA	2.18	0.43
2:F:44:ILE:HD12	2:F:44:ILE:H	1.81	0.43
2:E:40:GLN:HA	2:E:72:ARG:HD3	2.00	0.43
1:D:225:VAL:HG22	1:D:286:LEU:HD23	2.00	0.43
2:E:49:GLN:HG2	2:E:50:LEU:H	1.82	0.43
1:C:243:GLY:HA2	1:C:246:GLU:OE2	2.19	0.43
2:E:26:VAL:HG21	2:E:56:LEU:HD21	2.00	0.43
1:A:212:THR:HG22	1:A:213:LYS:N	2.27	0.42
2:H:56:LEU:HB3	2:H:61:ILE:HB	2.01	0.42
2:F:3:ILE:HG13	2:F:3:ILE:O	2.19	0.42
1:C:232:LEU:HG	1:C:296:ILE:HD12	2.02	0.42
2:F:7:THR:HG22	2:F:8:LEU:N	2.35	0.42
2:E:19:PRO:O	2:E:57:SER:HB2	2.20	0.41
1:D:215:LEU:C	1:D:217:THR:H	2.22	0.41
1:D:244:ASP:HB3	1:D:248:MSE:HE3	2.03	0.41
1:B:235:TYR:CD2	1:B:248:MSE:HE1	2.52	0.41
1:B:254:GLN:HA	1:B:254:GLN:OE1	2.21	0.41
2:H:63:LYS:O	2:H:64:GLU:CB	2.67	0.41
1:C:259:ARG:HG2	1:C:263:PHE:CE1	2.56	0.41
2:H:63:LYS:O	2:H:63:LYS:HG3	2.20	0.41
1:A:215:LEU:C	1:A:215:LEU:HD23	2.41	0.41
1:D:271:ASP:C	1:D:273:ASP:N	2.74	0.40
2:F:51:GLU:HB2	2:F:54:ARG:HH11	1.86	0.40
2:G:37:PRO:HA	2:G:38:PRO:HD3	1.89	0.40
2:G:1:MET:HB2	2:G:63:LYS:HB3	2.02	0.40
1:A:236:SER:HB3	1:A:239:ASP:HB2	2.02	0.40
2:F:44:ILE:N	2:F:44:ILE:CD1	2.77	0.40
2:F:7:THR:HG22	2:F:8:LEU:H	1.86	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	88/111 (79%)	79 (90%)	8 (9%)	1 (1%)	14 30
1	B	88/111 (79%)	82 (93%)	4 (4%)	2 (2%)	6 11
1	C	88/111 (79%)	88 (100%)	0	0	100 100
1	D	86/111 (78%)	78 (91%)	7 (8%)	1 (1%)	13 27
2	E	70/76 (92%)	69 (99%)	1 (1%)	0	100 100
2	F	71/76 (93%)	66 (93%)	5 (7%)	0	100 100
2	G	70/76 (92%)	67 (96%)	3 (4%)	0	100 100
2	H	72/76 (95%)	68 (94%)	4 (6%)	0	100 100
All	All	633/748 (85%)	597 (94%)	32 (5%)	4 (1%)	25 47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	301	VAL
1	B	303	ASN
1	A	299	GLY
1	B	239	ASP

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	85/101 (84%)	80 (94%)	5 (6%)	19 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	84/101 (83%)	76 (90%)	8 (10%)	8 16
1	C	85/101 (84%)	80 (94%)	5 (6%)	19 39
1	D	83/101 (82%)	74 (89%)	9 (11%)	6 12
2	E	66/68 (97%)	61 (92%)	5 (8%)	13 26
2	F	67/68 (98%)	63 (94%)	4 (6%)	19 39
2	G	66/68 (97%)	64 (97%)	2 (3%)	41 67
2	H	68/68 (100%)	64 (94%)	4 (6%)	19 39
All	All	604/676 (89%)	562 (93%)	42 (7%)	15 30

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	GLU
1	A	237	GLN
1	A	242	ASP
1	A	280	LEU
1	A	281	GLN
1	B	216	HIS
1	B	227	LEU
1	B	228	LEU
1	B	232	LEU
1	B	233	LEU
1	B	239	ASP
1	B	251	LEU
1	B	302	ILE
1	C	228	LEU
1	C	232	LEU
1	C	247	LEU
1	C	262	LEU
1	C	288	ARG
1	D	228	LEU
1	D	232	LEU
1	D	237	GLN
1	D	239	ASP
1	D	247	LEU
1	D	251	LEU
1	D	261	THR
1	D	265	LEU
1	D	289	VAL
2	E	16	GLU

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Mol	Chain	Res	Type
2	E	25	ASN
2	E	39	ASP
2	E	54	ARG
2	E	62	GLN
2	F	54	ARG
2	F	64	GLU
2	F	66	THR
2	F	69	LEU
2	G	63	LYS
2	G	64	GLU
2	H	15	LEU
2	H	34	GLU
2	H	39	ASP
2	H	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	285	ASN
1	A	291	ASN
1	B	222	ASN
1	B	223	ASN
1	B	237	GLN
1	B	285	ASN
1	B	291	ASN
1	B	300	GLN
1	C	222	ASN
1	C	224	ASN
1	C	291	ASN
1	D	234	HIS
1	D	237	GLN
1	D	254	GLN
1	D	272	ASN
1	D	285	ASN
1	D	300	GLN
2	E	2	GLN
2	E	25	ASN
2	E	40	GLN
2	E	60	ASN
2	E	62	GLN
2	F	25	ASN

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Mol	Chain	Res	Type
2	F	40	GLN
2	F	49	GLN
2	F	60	ASN
2	F	62	GLN
2	G	25	ASN
2	G	40	GLN
2	G	49	GLN
2	H	62	GLN
2	H	68	HIS

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	88/111 (79%)	0.55	10 (11%) 5 3	31, 61, 105, 108	0
1	B	88/111 (79%)	-0.36	0 100 100	27, 40, 80, 99	0
1	C	88/111 (79%)	-0.35	1 (1%) 80 78	23, 38, 65, 74	0
1	D	86/111 (77%)	-0.00	5 (5%) 23 17	31, 44, 92, 101	0
2	E	72/76 (94%)	-0.10	0 100 100	48, 69, 78, 86	0
2	F	73/76 (96%)	0.07	2 (2%) 54 48	38, 68, 79, 86	0
2	G	72/76 (94%)	-0.42	0 100 100	28, 44, 59, 64	0
2	H	74/76 (97%)	-0.49	0 100 100	27, 38, 51, 57	0
All	All	641/748 (85%)	-0.13	18 (2%) 53 46	23, 47, 84, 108	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	302	ILE	7.4
1	D	272	ASN	3.8
1	A	211	VAL	3.6
1	A	235	TYR	3.6
1	D	271	ASP	3.4
1	A	299	GLY	2.8
1	A	234	HIS	2.8
1	A	239	ASP	2.7
1	D	273	ASP	2.7
1	A	238	GLU	2.7
1	A	232	LEU	2.6
1	A	233	LEU	2.5
2	F	73	LEU	2.5
1	A	296	ILE	2.5
2	F	13	ILE	2.4
1	C	212	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	215	LEU	2.4
1	A	298	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.