Full wwPDB X-ray Structure Validation Report (i)

Feb 2, 2025 – 01:56 am GMT

PDB ID	:	9GFC
Title	:	HDM2 complexed with stapled peptide-like ligand
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Deposited on	:	2024-08-08
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

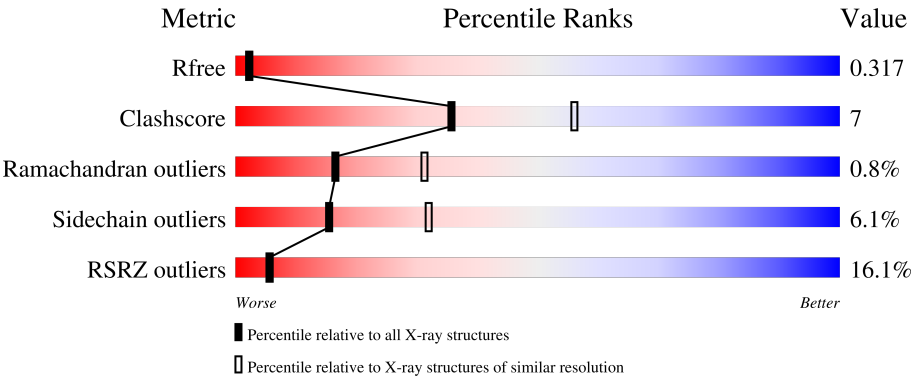
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	86	79% 20%
1	B	86	78% 20%
1	C	86	5% 76% 23%
1	D	86	62% 76% 22%
2	E	14	57% 29% 14%

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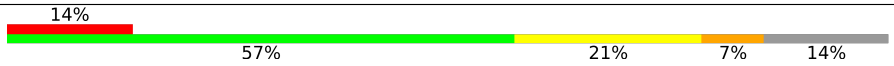
Mol	Chain	Length	Quality of chain
2	F	14	
2	G	14	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3180 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 E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			710	465	117	124	4			
1	B	86	Total	C	N	O	S	0	0	0
			703	462	116	121	4			
1	C	86	Total	C	N	O	S	0	0	0
			707	464	116	123	4			
1	D	86	Total	C	N	O	S	0	0	0
			696	458	113	121	4			

- Molecule 2 is a protein called Stapled peptide-like ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	0	0	1
			112	76	17	19			
2	F	13	Total	C	N	O	0	0	2
			104	71	16	17			
2	G	12	Total	C	N	O	0	0	1
			102	70	16	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	15	Total	O	0	0
			15	15		
3	C	9	Total	O	0	0
			9	9		
3	D	3	Total	O	0	0
			3	3		
3	E	5	Total	O	0	0
			5	5		

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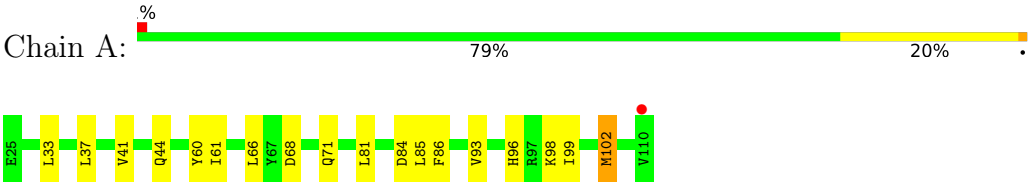
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	3	Total O 3 3	0	0
3	G	1	Total O 1 1	0	0

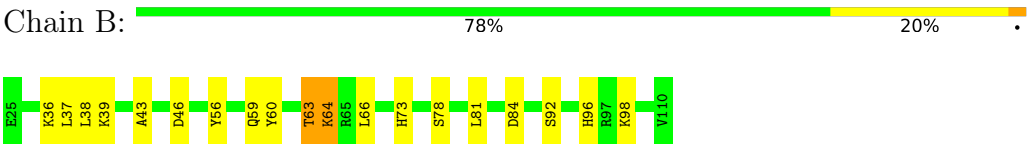
3 Residue-property plots (i)

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.

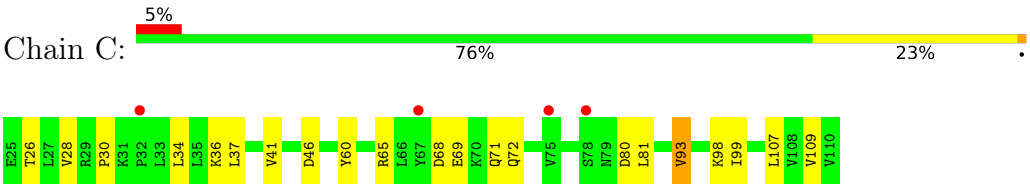
• Molecule 1: E3 ubiquitin-protein ligase Mdm2



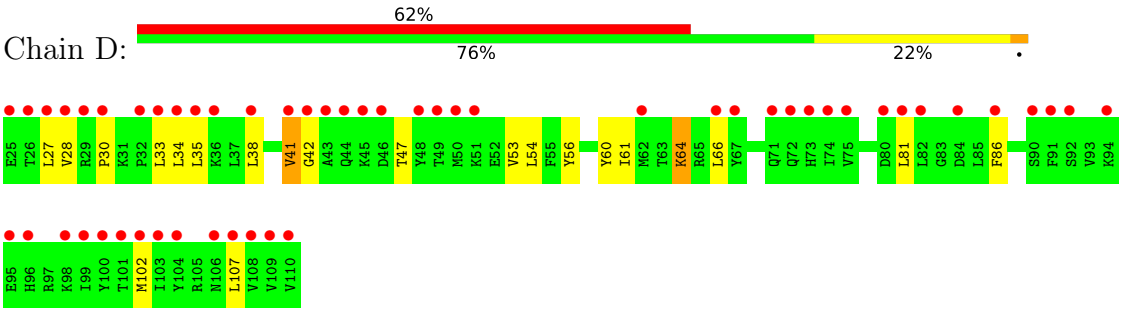
• Molecule 1: E3 ubiquitin-protein ligase Mdm2



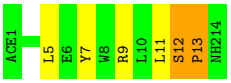
• Molecule 1: E3 ubiquitin-protein ligase Mdm2



• Molecule 1: E3 ubiquitin-protein ligase Mdm2

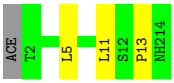


• Molecule 2: Stapled peptide-like ligand



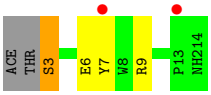
• Molecule 2: Stapled peptide-like ligand

Chain F:



• Molecule 2: Stapled peptide-like ligand

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.63Å 40.74Å 78.18Å 90.00° 95.86° 90.00°	Depositor
Resolution (Å)	28.13 – 2.50 28.13 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.13-2.50) 97.4 (28.13-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.263 , 0.318 0.255 , 0.317	Depositor DCC
R_{free} test set	644 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3180	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.68% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, HRG, NLE, ACE

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	0.39	0/724	0.57	0/975
1	B	0.38	0/717	0.59	0/966
1	C	0.35	0/721	0.53	0/971
1	D	0.30	0/710	0.50	0/958
2	E	0.23	0/91	0.57	0/122
2	F	0.23	0/85	0.51	0/112
2	G	0.21	0/83	0.49	0/110
All	All	0.35	0/3131	0.55	0/4214

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	1	1
2	G	0	1
All	All	1	2

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	12	SER	Peptide
2	G	3	SER	Peptide

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	710	0	742	13	0
1	B	703	0	734	10	0
1	C	707	0	738	8	0
1	D	696	0	721	11	0
2	E	112	0	105	7	0
2	F	104	0	95	3	0
2	G	102	0	94	3	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	9	0	0	0	0
3	D	3	0	0	0	0
3	E	5	0	0	0	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
All	All	3180	0	3229	46	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 7.

All (46) 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:73:HIS:HD1	1:B:92:SER:HG	1.15	0.94
1:A:96:HIS:CD2	2:E:11:LEU:HD23	2.28	0.69
1:B:96:HIS:CD2	2:F:11:LEU:HD23	2.29	0.68
1:A:81:LEU:HD22	1:B:36:LYS:HE3	1.75	0.68
1:C:30:PRO:HB3	1:C:34:LEU:HD23	1.80	0.62
1:C:36:LYS:HG3	1:C:81:LEU:HD21	1.82	0.60
1:D:42:GLY:HA2	2:F:5:NLE:HE2	1.83	0.60
1:B:64:LYS:HB3	1:B:66:LEU:HG	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:VAL:HG11	1:C:60:TYR:HA	1.86	0.58
1:A:37:LEU:HD12	1:A:81:LEU:HD23	1.88	0.56
1:D:41:VAL:HG11	1:D:60:TYR:HA	1.90	0.54
1:A:93:VAL:HG21	2:E:7:TYR:HB3	1.90	0.54
1:B:38:LEU:HD22	1:B:56:TYR:HB2	1.90	0.53
1:C:93:VAL:HA	1:C:99:ILE:HD11	1.91	0.53
1:B:37:LEU:HD11	1:B:81:LEU:HB3	1.91	0.53
1:C:28:VAL:HG12	1:C:109:VAL:HG22	1.91	0.52
1:D:27:LEU:HD22	1:D:47:THR:HG22	1.92	0.52
1:A:41:VAL:HG11	1:A:60:TYR:HA	1.93	0.51
1:A:33:LEU:HD11	1:A:81:LEU:HG	1.95	0.49
1:C:28:VAL:HG21	1:C:107:LEU:HD22	1.95	0.48
1:D:38:LEU:HD11	1:D:53:VAL:HG13	1.94	0.48
1:A:85:LEU:HG	1:A:102:MET:HG3	1.95	0.48
1:D:64:LYS:HB3	1:D:66:LEU:HG	1.96	0.47
2:G:9:HRG:HN21	2:G:9:HRG:HG1	1.79	0.47
1:A:86:PHE:HE2	1:A:98:LYS:HE3	1.80	0.46
1:D:61:ILE:HG23	1:D:66:LEU:HB2	1.97	0.46
1:D:28:VAL:HG21	1:D:107:LEU:HD22	1.97	0.46
1:A:61:ILE:HG23	1:A:66:LEU:HB2	1.98	0.45
1:D:30:PRO:HB3	1:D:34:LEU:HD23	1.98	0.45
1:B:59:GLN:O	1:B:63:THR:HB	2.17	0.45
1:D:86:PHE:CE1	1:D:102:MET:SD	3.11	0.44
1:B:96:HIS:CD2	2:F:11:LEU:CD2	3.00	0.44
2:G:3:SER:HA	2:G:6:GLU:HG2	1.99	0.44
1:C:68:ASP:HB3	1:C:71:GLN:O	2.18	0.43
1:B:60:TYR:O	1:B:64:LYS:HB2	2.19	0.43
2:E:12:SER:HA	2:E:13:PRO:O	2.19	0.43
1:A:68:ASP:HB3	1:A:71:GLN:O	2.18	0.43
1:D:33:LEU:HD11	1:D:81:LEU:HG	2.00	0.43
2:E:12:SER:HB2	2:E:13:PRO:HA	2.00	0.43
1:A:93:VAL:HA	1:A:99:ILE:HD11	2.00	0.42
1:A:93:VAL:CG2	2:E:7:TYR:HB3	2.48	0.42
1:D:38:LEU:HD22	1:D:56:TYR:HB3	2.02	0.41
2:E:5:NLE:HE3	2:E:9:HRG:HNE	1.72	0.40
1:A:96:HIS:CD2	2:E:11:LEU:CD2	3.00	0.40
1:B:39:LYS:HA	1:B:43:ALA:O	2.22	0.40
1:C:93:VAL:CG2	2:G:7:TYR:HB3	2.52	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	84/86 (98%)	81 (96%)	3 (4%)	0	100 100
1	B	84/86 (98%)	79 (94%)	5 (6%)	0	100 100
1	C	84/86 (98%)	78 (93%)	5 (6%)	1 (1%)	11 21
1	D	84/86 (98%)	78 (93%)	6 (7%)	0	100 100
2	E	10/14 (71%)	9 (90%)	0	1 (10%)	0 0
2	F	9/14 (64%)	8 (89%)	0	1 (11%)	0 0
2	G	8/14 (57%)	8 (100%)	0	0	100 100
All	All	363/386 (94%)	341 (94%)	19 (5%)	3 (1%)	16 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	13	PRO
2	F	13	PRO
1	C	72	GLN

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	80/81 (99%)	77 (96%)	3 (4%)	28 53
1	B	78/81 (96%)	72 (92%)	6 (8%)	10 22
1	C	79/81 (98%)	71 (90%)	8 (10%)	6 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	77/81 (95%)	73 (95%)	4 (5%)	19 39
2	E	10/10 (100%)	10 (100%)	0	100 100
2	F	9/10 (90%)	9 (100%)	0	100 100
2	G	9/10 (90%)	9 (100%)	0	100 100
All	All	342/354 (97%)	321 (94%)	21 (6%)	15 32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	84	ASP
1	A	102	MET
1	B	46	ASP
1	B	63	THR
1	B	64	LYS
1	B	78	SER
1	B	84	ASP
1	B	98	LYS
1	C	26	THR
1	C	37	LEU
1	C	46	ASP
1	C	65	ARG
1	C	69	GLU
1	C	80	ASP
1	C	93	VAL
1	C	98	LYS
1	D	35	LEU
1	D	41	VAL
1	D	54	LEU
1	D	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	D	79	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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HRG	G	9	2	10,11,12	0.42	0	6,12,14	0.61	0
2	NLE	E	5	2	6,7,8	0.55	0	2,7,9	0.16	0
2	NLE	G	5	2	6,7,8	0.54	0	2,7,9	0.06	0
2	NLE	F	5	2	6,7,8	0.50	0	2,7,9	0.23	0
2	HRG	F	9	2	10,11,12	0.39	0	6,12,14	0.59	0
2	HRG	E	9	2	10,11,12	0.39	0	6,12,14	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HRG	G	9	2	-	2/9/10/12	-
2	NLE	E	5	2	-	1/5/6/8	-
2	NLE	G	5	2	-	3/5/6/8	-
2	NLE	F	5	2	-	3/5/6/8	-
2	HRG	F	9	2	-	2/9/10/12	-
2	HRG	E	9	2	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	NLE	O-C-CA-CB
2	F	5	NLE	O-C-CA-CB
2	G	5	NLE	N-CA-CB-CG
2	G	5	NLE	C-CA-CB-CG
2	G	9	HRG	CG-CD-NE-CZ
2	F	5	NLE	CA-CB-CG-CD
2	F	9	HRG	CD-CG-CG'-CB
2	E	9	HRG	CD-CG-CG'-CB
2	F	9	HRG	C-CA-CB-CG'
2	G	5	NLE	CA-CB-CG-CD
2	F	5	NLE	N-CA-CB-CG
2	E	9	HRG	C-CA-CB-CG'
2	G	9	HRG	C-CA-CB-CG'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	9	HRG	1	0
2	E	5	NLE	1	0
2	F	5	NLE	1	0
2	E	9	HRG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	86/86 (100%)	0.10	1 (1%) 76 73	9, 18, 31, 37	0
1	B	86/86 (100%)	0.17	0 100 100	11, 19, 29, 35	0
1	C	86/86 (100%)	0.96	4 (4%) 37 34	26, 40, 46, 49	0
1	D	86/86 (100%)	2.26	53 (61%) 0 0	38, 61, 69, 73	0
2	E	10/14 (71%)	0.52	0 100 100	15, 22, 29, 33	0
2	F	10/14 (71%)	0.22	0 100 100	18, 23, 27, 28	0
2	G	9/14 (64%)	1.61	2 (22%) 3 3	39, 39, 41, 43	0
All	All	373/386 (96%)	0.86	60 (16%) 5 6	9, 30, 67, 73	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	LEU	4.9
1	D	108	VAL	4.7
1	D	110	VAL	4.4
1	D	30	PRO	4.1
1	D	46	ASP	4.1
1	D	81	LEU	4.0
1	C	32	PRO	3.9
1	D	66	LEU	3.5
1	D	103	ILE	3.5
1	D	100	TYR	3.4
1	D	95	GLU	3.4
1	D	28	VAL	3.3
1	D	26	THR	3.2
1	D	43	ALA	3.1
1	D	32	PRO	3.1
1	D	41	VAL	3.0
1	D	109	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	106	ASN	2.9
1	D	86	PHE	2.9
1	D	84	ASP	2.9
1	D	62	MET	2.8
1	D	107	LEU	2.8
1	D	94	LYS	2.8
1	D	104	TYR	2.8
1	D	35	LEU	2.7
1	D	91	PHE	2.7
1	D	98	LYS	2.7
2	G	13	PRO	2.6
1	D	33	LEU	2.6
1	D	34	LEU	2.6
1	D	29	ARG	2.6
1	D	101	THR	2.6
1	D	38	LEU	2.5
1	D	72	GLN	2.5
1	D	75	VAL	2.5
1	D	90	SER	2.4
1	D	45	LYS	2.4
1	D	48	TYR	2.4
1	A	110	VAL	2.4
1	D	99	ILE	2.4
1	D	50	MET	2.3
1	C	75	VAL	2.3
1	D	80	ASP	2.2
1	D	96	HIS	2.2
1	D	49	THR	2.2
1	D	67	TYR	2.2
1	C	78	SER	2.2
1	D	74	ILE	2.2
1	D	82	LEU	2.2
1	D	25	GLU	2.1
1	D	42	GLY	2.1
1	D	102	MET	2.1
1	D	44	GLN	2.1
1	D	51	LYS	2.1
2	G	7	TYR	2.1
1	D	36	LYS	2.0
1	C	67	TYR	2.0
1	D	71	GLN	2.0
1	D	73	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	92	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HRG	G	9	12/13	0.76	0.14	39,40,41,41	0
2	NLE	G	5	8/9	0.77	0.13	41,41,42,42	0
2	NLE	E	5	8/9	0.79	0.14	20,21,21,22	0
2	NLE	F	5	8/9	0.79	0.11	23,25,26,27	0
2	HRG	F	9	12/13	0.86	0.12	20,22,27,27	0
2	HRG	E	9	12/13	0.87	0.11	17,17,18,19	0

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.