Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:57 am BST

PDB ID	:	5MNJ
Title	:	Structure of MDM2-MDMX-UbcH5B-ubiquitin complex
Authors	:	Klejnot, M.; Huang, D.T.
Deposited on	:	2016-12-13
Resolution	:	2.16 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:

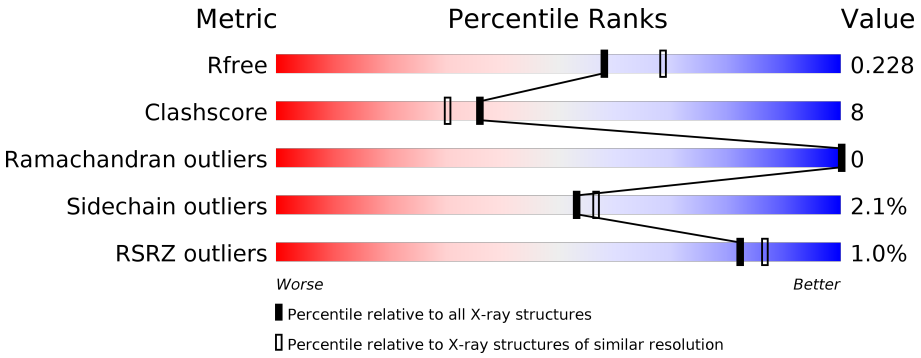
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	147	% 85% 14% ·
1	E	147	81% 18% ··
2	B	81	5% 70% 21% · 7%
2	F	81	81% 12% 6%
3	C	86	% 63% 10% 27%
3	G	86	63% 12% · 24%

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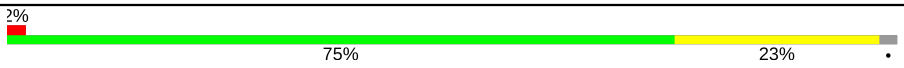
Mol	Chain	Length	Quality of chain
4	D	64	
4	H	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	H	503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5413 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 Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	2	0
			1146	744	198	198	6			
1	E	146	Total	C	N	O	S	0	2	0
			1157	749	197	205	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	SER	engineered mutation	UNP P62837
A	85	LYS	CYS	engineered mutation	UNP P62837
E	22	ARG	SER	engineered mutation	UNP P62837
E	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O		0	0	0
			527	337	91	99				
2	F	76	Total	C	N	O	S	0	0	0
			570	361	101	107	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P0CG47
B	-3	SER	-	expression tag	UNP P0CG47
B	-2	GLY	-	expression tag	UNP P0CG47
B	-1	GLY	-	expression tag	UNP P0CG47
B	0	SER	-	expression tag	UNP P0CG47
F	-4	GLY	-	expression tag	UNP P0CG47
F	-3	SER	-	expression tag	UNP P0CG47
F	-2	GLY	-	expression tag	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P0CG47
F	0	SER	-	expression tag	UNP P0CG47

- Molecule 3 is a protein called E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	63	Total	C	N	O	S	0	0	0
			471	300	86	76	9			
3	G	65	Total	C	N	O	S	0	0	0
			485	309	89	78	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	406	MET	-	initiating methionine	UNP Q00987
C	407	GLY	-	expression tag	UNP Q00987
C	408	SER	-	expression tag	UNP Q00987
C	409	SER	-	expression tag	UNP Q00987
C	410	HIS	-	expression tag	UNP Q00987
C	411	HIS	-	expression tag	UNP Q00987
C	412	HIS	-	expression tag	UNP Q00987
C	413	HIS	-	expression tag	UNP Q00987
C	414	HIS	-	expression tag	UNP Q00987
C	415	HIS	-	expression tag	UNP Q00987
C	416	SER	-	expression tag	UNP Q00987
C	417	GLN	-	expression tag	UNP Q00987
C	418	ASP	-	expression tag	UNP Q00987
C	419	LEU	-	expression tag	UNP Q00987
C	420	GLU	-	expression tag	UNP Q00987
C	421	ASN	-	expression tag	UNP Q00987
C	422	LEU	-	expression tag	UNP Q00987
C	423	TYR	-	expression tag	UNP Q00987
C	424	PHE	-	expression tag	UNP Q00987
C	425	GLN	-	expression tag	UNP Q00987
C	426	GLY	-	expression tag	UNP Q00987
C	427	SER	-	expression tag	UNP Q00987
G	406	MET	-	initiating methionine	UNP Q00987
G	407	GLY	-	expression tag	UNP Q00987
G	408	SER	-	expression tag	UNP Q00987
G	409	SER	-	expression tag	UNP Q00987
G	410	HIS	-	expression tag	UNP Q00987
G	411	HIS	-	expression tag	UNP Q00987

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Chain	Residue	Modelled	Actual	Comment	Reference
G	412	HIS	-	expression tag	UNP Q00987
G	413	HIS	-	expression tag	UNP Q00987
G	414	HIS	-	expression tag	UNP Q00987
G	415	HIS	-	expression tag	UNP Q00987
G	416	SER	-	expression tag	UNP Q00987
G	417	GLN	-	expression tag	UNP Q00987
G	418	ASP	-	expression tag	UNP Q00987
G	419	LEU	-	expression tag	UNP Q00987
G	420	GLU	-	expression tag	UNP Q00987
G	421	ASN	-	expression tag	UNP Q00987
G	422	LEU	-	expression tag	UNP Q00987
G	423	TYR	-	expression tag	UNP Q00987
G	424	PHE	-	expression tag	UNP Q00987
G	425	GLN	-	expression tag	UNP Q00987
G	426	GLY	-	expression tag	UNP Q00987
G	427	SER	-	expression tag	UNP Q00987

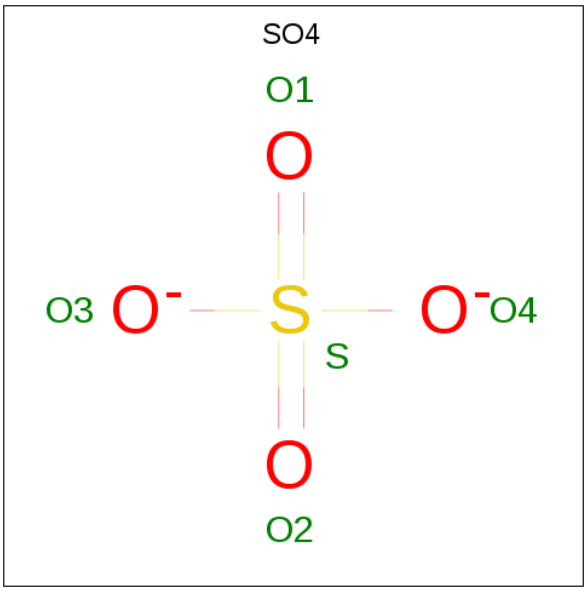
- Molecule 4 is a protein called Protein Mdm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			475	300	92	77	6			
4	H	64	Total	C	N	O	S	0	0	0
			487	306	94	80	7			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	2	Total	Zn	0	0
			2	2		
5	G	2	Total	Zn	0	0
			2	2		
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

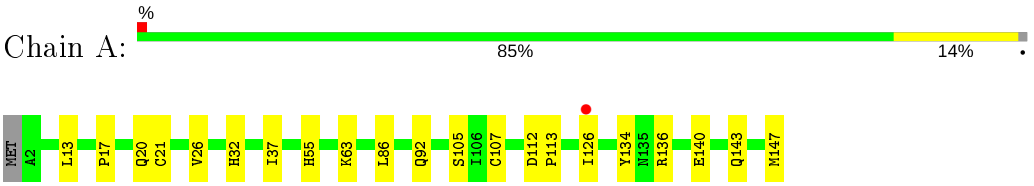
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	B	4	Total O 4 4	0	0
7	C	2	Total O 2 2	0	0
7	D	7	Total O 7 7	0	0
7	E	27	Total O 27 27	0	0
7	F	5	Total O 5 5	0	0
7	G	11	Total O 11 11	0	0
7	H	8	Total O 8 8	0	0

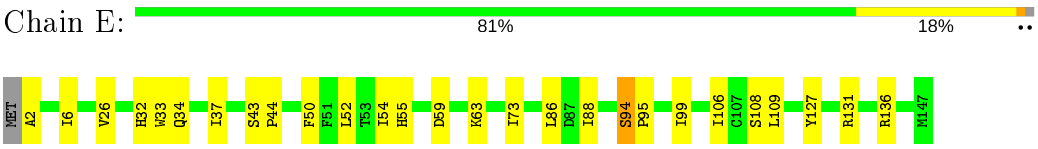
3 Residue-property plots

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.

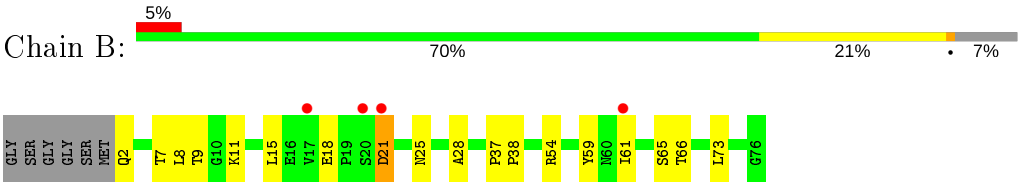
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2



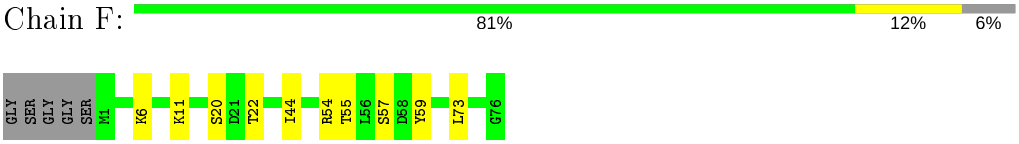
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2



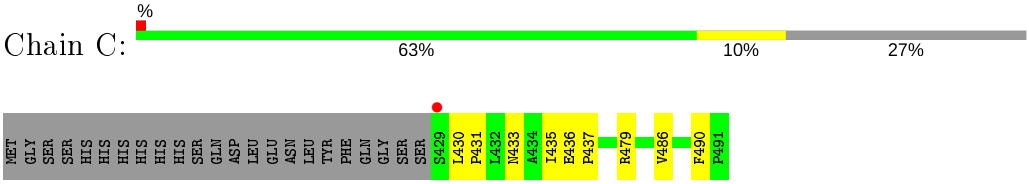
- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B

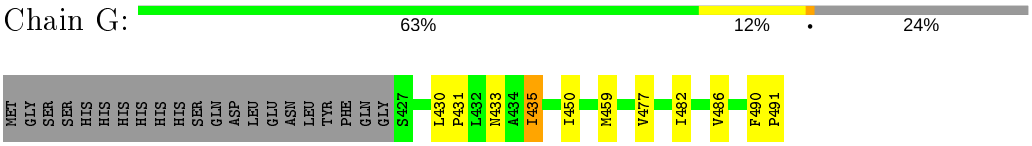


- Molecule 3: E3 ubiquitin-protein ligase Mdm2



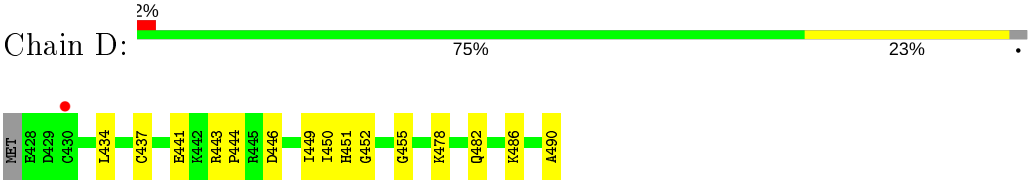
- Molecule 3: E3 ubiquitin-protein ligase Mdm2

Chain G:



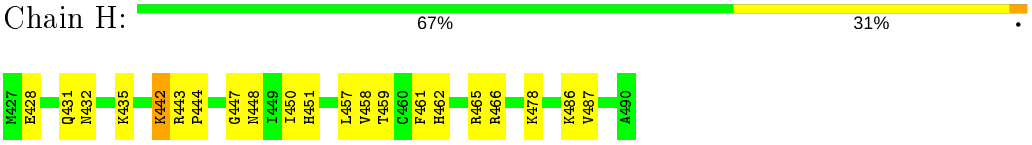
• Molecule 4: Protein Mdm4

Chain D:



• Molecule 4: Protein Mdm4

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.24Å 62.76Å 66.35Å 69.83° 69.22° 78.21°	Depositor
Resolution (Å)	50.49 – 2.16 50.49 – 2.16	Depositor EDS
% Data completeness (in resolution range)	92.4 (50.49-2.16) 93.6 (50.49-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.190 , 0.231 0.188 , 0.228	Depositor DCC
R_{free} test set	1928 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5413	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: ZN, SO4

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	0.41	0/1190	0.61	0/1627
1	E	0.42	0/1201	0.61	0/1641
2	B	0.33	0/533	0.51	0/728
2	F	0.38	0/576	0.56	0/779
3	C	0.46	0/482	0.62	0/653
3	G	0.45	0/496	0.63	0/672
4	D	0.44	0/482	0.64	0/646
4	H	0.44	0/494	0.63	0/661
All	All	0.42	0/5454	0.60	0/7407

There are no bond length outliers.

There are no bond angle outliers.

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	1146	0	1115	18	0
1	E	1157	0	1127	18	0
2	B	527	0	500	14	0
2	F	570	0	581	7	0
3	C	471	0	477	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	485	0	495	8	0
4	D	475	0	493	9	0
4	H	487	0	506	17	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	D	5	0	0	0	0
6	H	5	0	0	3	0
7	A	13	0	0	0	0
7	B	4	0	0	0	0
7	C	2	0	0	0	0
7	D	7	0	0	0	0
7	E	27	0	0	3	0
7	F	5	0	0	0	0
7	G	11	0	0	0	0
7	H	8	0	0	1	0
All	All	5413	0	5294	85	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 8.

All (85) 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)
4:H:442:LYS:NZ	6:H:503:SO4:O2	2.06	0.89
4:H:466:ARG:NH2	6:H:503:SO4:O4	2.09	0.85
1:E:26:VAL:HG22	1:E:34:GLN:HB2	1.65	0.78
3:G:430:LEU:HB3	3:G:431:PRO:HD3	1.75	0.67
2:B:9:THR:HG21	4:D:490:ALA:HB1	1.78	0.65
1:A:126:ILE:HG22	1:A:134:TYR:HB2	1.80	0.64
1:A:32[B]:HIS:CD2	1:A:55[B]:HIS:NE2	2.67	0.62
1:E:108:SER:HB3	2:F:44:ILE:HD12	1.82	0.62
1:A:32[B]:HIS:HD2	1:A:55[B]:HIS:NE2	1.98	0.61
4:H:428:GLU:O	4:H:431:GLN:HG2	2.00	0.61
1:A:136:ARG:NH1	1:A:140:GLU:OE2	2.34	0.61
1:A:20:GLN:O	1:A:21:CYS:SG	2.57	0.61
2:B:7:THR:HG22	2:B:8:LEU:N	2.16	0.61
1:A:13:LEU:O	1:A:17:PRO:HG3	2.01	0.60
2:F:11:LYS:HD3	3:G:433:ASN:ND2	2.17	0.60
4:H:461:PHE:CZ	4:H:465:ARG:HD3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB3	2:B:73:LEU:CD2	2.34	0.57
1:E:136:ARG:HG2	7:E:211:HOH:O	2.05	0.57
1:A:37:ILE:HG23	1:A:107:CYS:SG	2.44	0.56
2:B:18:GLU:O	2:B:21:ASP:HB2	2.04	0.56
1:A:32[B]:HIS:HD2	1:A:55[B]:HIS:CD2	2.24	0.55
1:E:55[B]:HIS:HD2	7:E:203:HOH:O	1.90	0.55
4:H:442:LYS:NZ	6:H:503:SO4:S	2.80	0.54
2:B:61:ILE:HG23	2:B:65:SER:OG	2.08	0.53
1:E:43:SER:HB2	1:E:44:PRO:HD2	1.89	0.53
2:B:2:GLN:HA	2:B:15:LEU:O	2.07	0.53
1:E:32[A]:HIS:NE2	1:E:55[A]:HIS:CD2	2.77	0.53
2:F:54:ARG:HD2	2:F:59:TYR:OH	2.09	0.53
4:H:447:GLY:O	4:H:457:LEU:HD12	2.08	0.53
1:E:37:ILE:HD12	1:E:52:LEU:HD11	1.92	0.51
1:E:2:ALA:O	1:E:6:ILE:HG13	2.10	0.50
2:F:73:LEU:HD12	2:F:73:LEU:C	2.32	0.50
4:D:443:ARG:HB3	4:D:444:PRO:HD2	1.93	0.49
3:G:450:ILE:HG23	3:G:482:ILE:HG23	1.93	0.49
2:B:61:ILE:O	2:B:61:ILE:HG22	2.11	0.49
2:B:7:THR:CG2	2:B:8:LEU:N	2.76	0.49
1:A:26:VAL:HG23	1:A:26:VAL:O	2.13	0.48
3:C:486:VAL:HG21	4:D:450:ILE:HD13	1.94	0.48
1:E:32[B]:HIS:CD2	1:E:55[B]:HIS:CE1	3.01	0.48
4:H:432:ASN:HA	4:H:435:LYS:HD2	1.94	0.48
2:B:7:THR:HB	2:B:11:LYS:HG2	1.96	0.47
4:D:437:CYS:O	4:D:441:GLU:HG3	2.15	0.47
1:A:134:TYR:C	1:A:134:TYR:CD1	2.87	0.47
2:F:6:LYS:HB3	2:F:6:LYS:HE3	1.59	0.47
1:A:92:GLN:HB3	3:C:479:ARG:NH2	2.30	0.46
3:G:459:MET:SD	3:G:477:VAL:HG23	2.55	0.46
3:C:436:GLU:HG2	3:C:437:PRO:HD2	1.97	0.46
1:E:33:TRP:HB2	1:E:54:ILE:HB	1.96	0.46
4:H:478:LYS:HA	4:H:478:LYS:HD3	1.75	0.46
2:F:54:ARG:HD2	2:F:59:TYR:CZ	2.51	0.46
2:B:54:ARG:CB	2:B:59:TYR:CE2	2.99	0.46
1:E:99:ILE:HA	1:E:99:ILE:HD13	1.79	0.46
3:G:491:PRO:HD2	4:H:458:VAL:CG1	2.46	0.46
1:A:63:LYS:HA	1:A:63:LYS:HD2	1.79	0.46
4:D:449:ILE:O	4:D:455:GLY:HA2	2.16	0.46
4:H:458:VAL:HG23	4:H:459:THR:HG23	1.98	0.45
1:E:55[B]:HIS:CD2	7:E:203:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:452:GLY:N	4:D:482:GLN:OE1	2.35	0.44
3:G:491:PRO:HD2	4:H:458:VAL:HG13	2.00	0.44
1:A:112:ASP:N	1:A:113:PRO:HD3	2.32	0.44
1:A:86:LEU:HD11	2:B:73:LEU:HD13	1.99	0.44
3:C:435:ILE:HD11	4:D:434:LEU:HD11	1.99	0.44
2:B:25:ASN:O	2:B:28:ALA:HB3	2.17	0.44
3:C:430:LEU:N	3:C:431:PRO:CD	2.81	0.44
1:A:26:VAL:CG2	1:A:26:VAL:O	2.66	0.43
3:G:435:ILE:CD1	3:G:435:ILE:N	2.82	0.43
4:H:486:LYS:NZ	7:H:602:HOH:O	2.51	0.43
1:E:106:ILE:O	1:E:109:LEU:HB3	2.19	0.43
3:C:435:ILE:HG22	3:C:435:ILE:O	2.18	0.43
4:H:443:ARG:HB3	4:H:444:PRO:HD2	2.01	0.43
3:G:486:VAL:HG21	4:H:450:ILE:HD13	2.02	0.42
4:H:462:HIS:O	4:H:466:ARG:HD3	2.20	0.42
4:D:478:LYS:HA	4:D:478:LYS:HD2	1.70	0.42
4:H:448:ASN:HB2	4:H:487:VAL:CG2	2.50	0.41
1:A:105:SER:HB3	2:B:73:LEU:HD22	2.02	0.41
4:D:446:ASP:OD2	4:D:486:LYS:NZ	2.53	0.41
1:E:59:ASP:OD2	1:E:63:LYS:HG2	2.20	0.41
1:E:94:SER:HA	1:E:95:PRO:HD3	1.93	0.41
2:F:22:THR:HA	2:F:55:THR:HA	2.01	0.41
1:E:127:TYR:O	1:E:131:ARG:NE	2.37	0.41
1:A:143:GLN:O	1:A:147:MET:HG3	2.20	0.40
1:E:50:PHE:CE2	1:E:73:ILE:HD12	2.56	0.40
2:B:37:PRO:HA	2:B:38:PRO:HD3	1.92	0.40
4:H:461:PHE:CE2	4:H:465:ARG:HD3	2.57	0.40
1:E:86:LEU:HG	1:E:88:ILE:HG12	2.03	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	146/147 (99%)	139 (95%)	7 (5%)	0	100	100
1	E	146/147 (99%)	142 (97%)	4 (3%)	0	100	100
2	B	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
2	F	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
3	C	61/86 (71%)	57 (93%)	4 (7%)	0	100	100
3	G	63/86 (73%)	61 (97%)	2 (3%)	0	100	100
4	D	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	H	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
All	All	686/756 (91%)	662 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	121/131 (92%)	121 (100%)	0	100	100
1	E	125/131 (95%)	124 (99%)	1 (1%)	81	86
2	B	49/70 (70%)	47 (96%)	2 (4%)	30	29
2	F	60/70 (86%)	58 (97%)	2 (3%)	38	37
3	C	52/77 (68%)	50 (96%)	2 (4%)	33	31
3	G	54/77 (70%)	52 (96%)	2 (4%)	34	32
4	D	51/56 (91%)	50 (98%)	1 (2%)	55	59
4	H	53/56 (95%)	51 (96%)	2 (4%)	33	31
All	All	565/668 (85%)	553 (98%)	12 (2%)	53	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	21	ASP
2	B	66	THR

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Mol	Chain	Res	Type
3	C	433	ASN
3	C	490	PHE
4	D	451	HIS
1	E	94	SER
2	F	20	SER
2	F	57	SER
3	G	435	ILE
3	G	490	PHE
4	H	442	LYS
4	H	451	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	433	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
6	SO4	D	503	-	4,4,4	0.17	0	6,6,6	0.22	0
6	SO4	H	503	-	4,4,4	0.19	0	6,6,6	0.34	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	503	SO4	3	0

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	146/147 (99%)	0.17	1 (0%) 87 91	38, 53, 83, 90	0
1	E	146/147 (99%)	-0.01	0 100 100	38, 49, 68, 80	0
2	B	75/81 (92%)	0.24	4 (5%) 26 35	45, 65, 98, 107	0
2	F	76/81 (93%)	0.04	0 100 100	39, 59, 77, 80	0
3	C	63/86 (73%)	0.10	1 (1%) 72 77	40, 51, 68, 79	0
3	G	65/86 (75%)	0.17	0 100 100	38, 49, 72, 90	0
4	D	63/64 (98%)	0.10	1 (1%) 72 77	40, 47, 61, 72	0
4	H	64/64 (100%)	-0.00	0 100 100	37, 45, 64, 78	0
All	All	698/756 (92%)	0.10	7 (1%) 82 86	37, 52, 80, 107	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	17	VAL	3.4
2	B	20	SER	3.3
4	D	430	CYS	2.8
1	A	126	ILE	2.2
2	B	21	ASP	2.2
2	B	61	ILE	2.1
3	C	429	SER	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

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
6	SO4	H	503	5/5	0.98	0.12	58,59,62,65	0
6	SO4	D	503	5/5	0.99	0.11	47,49,53,54	0
5	ZN	C	501	1/1	0.99	0.15	52,52,52,52	0
5	ZN	G	501	1/1	0.99	0.13	48,48,48,48	0
5	ZN	C	502	1/1	0.99	0.15	48,48,48,48	0
5	ZN	D	501	1/1	0.99	0.11	43,43,43,43	0
5	ZN	H	501	1/1	1.00	0.15	40,40,40,40	0
5	ZN	G	502	1/1	1.00	0.17	41,41,41,41	0
5	ZN	D	502	1/1	1.00	0.14	45,45,45,45	0
5	ZN	H	502	1/1	1.00	0.14	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.