



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:52 AM UTC

PDB ID : 8HSV / pdb_00008hsv
Title : The structure of rat beta-arrestin1 in complex with a rat Mdm2 peptide
Authors : Yun, Y.; Yoon, H.J.; Choi, Y.; Lee, H.H.
Deposited on : 2022-12-20
Resolution : 3.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

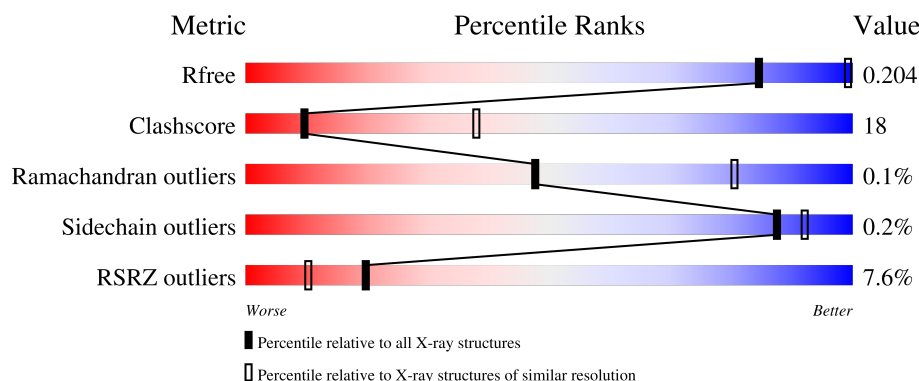
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	414	5% 55% 32% • 12%
1	B	414	5% 56% 31% • 12%
2	E	18	56% 56% 22% 6% 17%
2	F	18	33% 50% 6% 44%

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
3	SO4	A	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6042 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2881	1841	497	540	3			
1	B	363	Total	C	N	O	S	0	0	0
			2867	1833	489	542	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P29066
A	-18	GLY	-	expression tag	UNP P29066
A	-17	SER	-	expression tag	UNP P29066
A	-16	SER	-	expression tag	UNP P29066
A	-15	HIS	-	expression tag	UNP P29066
A	-14	HIS	-	expression tag	UNP P29066
A	-13	HIS	-	expression tag	UNP P29066
A	-12	HIS	-	expression tag	UNP P29066
A	-11	HIS	-	expression tag	UNP P29066
A	-10	HIS	-	expression tag	UNP P29066
A	-9	SER	-	expression tag	UNP P29066
A	-8	SER	-	expression tag	UNP P29066
A	-7	GLY	-	expression tag	UNP P29066
A	-6	LEU	-	expression tag	UNP P29066
A	-5	VAL	-	expression tag	UNP P29066
A	-4	PRO	-	expression tag	UNP P29066
A	-3	ARG	-	expression tag	UNP P29066
A	-2	GLY	-	expression tag	UNP P29066
A	-1	SER	-	expression tag	UNP P29066
A	0	HIS	-	expression tag	UNP P29066
A	59	VAL	CYS	engineered mutation	UNP P29066
A	125	SER	CYS	engineered mutation	UNP P29066
A	140	LEU	CYS	engineered mutation	UNP P29066
A	150	VAL	CYS	engineered mutation	UNP P29066
A	242	VAL	CYS	engineered mutation	UNP P29066

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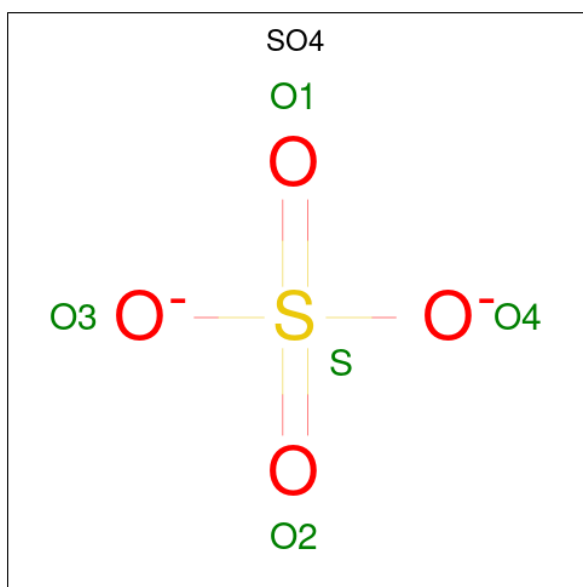
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Chain	Residue	Modelled	Actual	Comment	Reference
A	251	VAL	CYS	engineered mutation	UNP P29066
A	269	SER	CYS	engineered mutation	UNP P29066
B	-19	MET	-	initiating methionine	UNP P29066
B	-18	GLY	-	expression tag	UNP P29066
B	-17	SER	-	expression tag	UNP P29066
B	-16	SER	-	expression tag	UNP P29066
B	-15	HIS	-	expression tag	UNP P29066
B	-14	HIS	-	expression tag	UNP P29066
B	-13	HIS	-	expression tag	UNP P29066
B	-12	HIS	-	expression tag	UNP P29066
B	-11	HIS	-	expression tag	UNP P29066
B	-10	HIS	-	expression tag	UNP P29066
B	-9	SER	-	expression tag	UNP P29066
B	-8	SER	-	expression tag	UNP P29066
B	-7	GLY	-	expression tag	UNP P29066
B	-6	LEU	-	expression tag	UNP P29066
B	-5	VAL	-	expression tag	UNP P29066
B	-4	PRO	-	expression tag	UNP P29066
B	-3	ARG	-	expression tag	UNP P29066
B	-2	GLY	-	expression tag	UNP P29066
B	-1	SER	-	expression tag	UNP P29066
B	0	HIS	-	expression tag	UNP P29066
B	59	VAL	CYS	engineered mutation	UNP P29066
B	125	SER	CYS	engineered mutation	UNP P29066
B	140	LEU	CYS	engineered mutation	UNP P29066
B	150	VAL	CYS	engineered mutation	UNP P29066
B	242	VAL	CYS	engineered mutation	UNP P29066
B	251	VAL	CYS	engineered mutation	UNP P29066
B	269	SER	CYS	engineered mutation	UNP P29066

- Molecule 2 is a protein called peptide from E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	15	Total	C	N	O	S	0	0	0
			109	62	18	28	1			
2	F	10	Total	C	N	O	S	0	0	0
			72	40	11	20	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

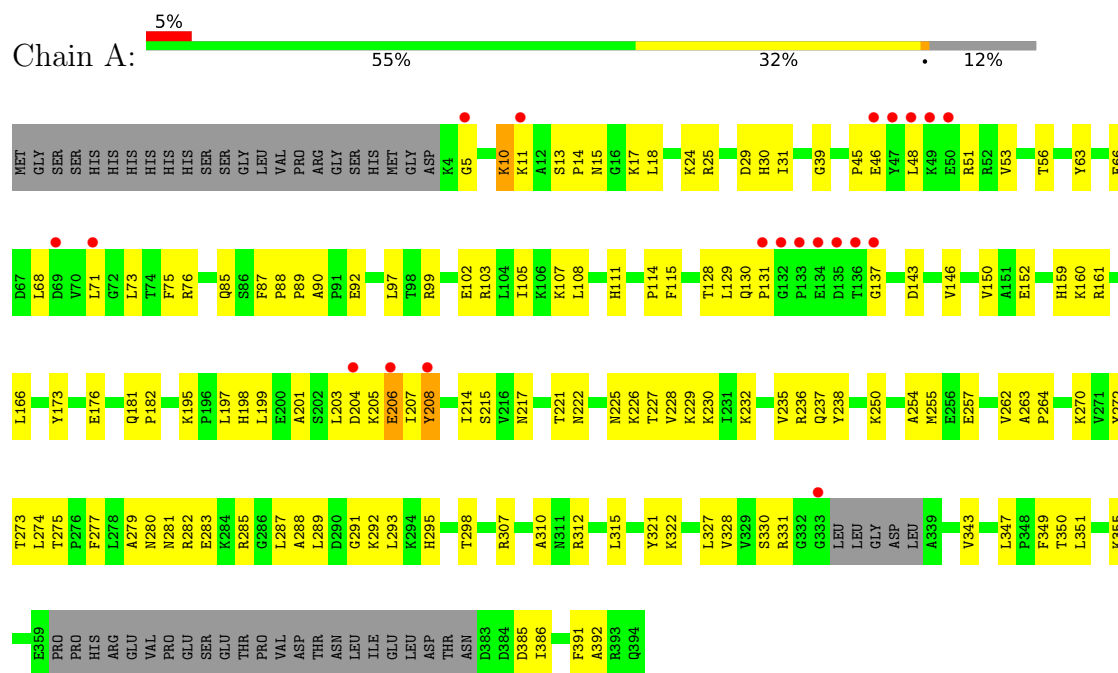
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	47	Total	O	0	0
			47	47		

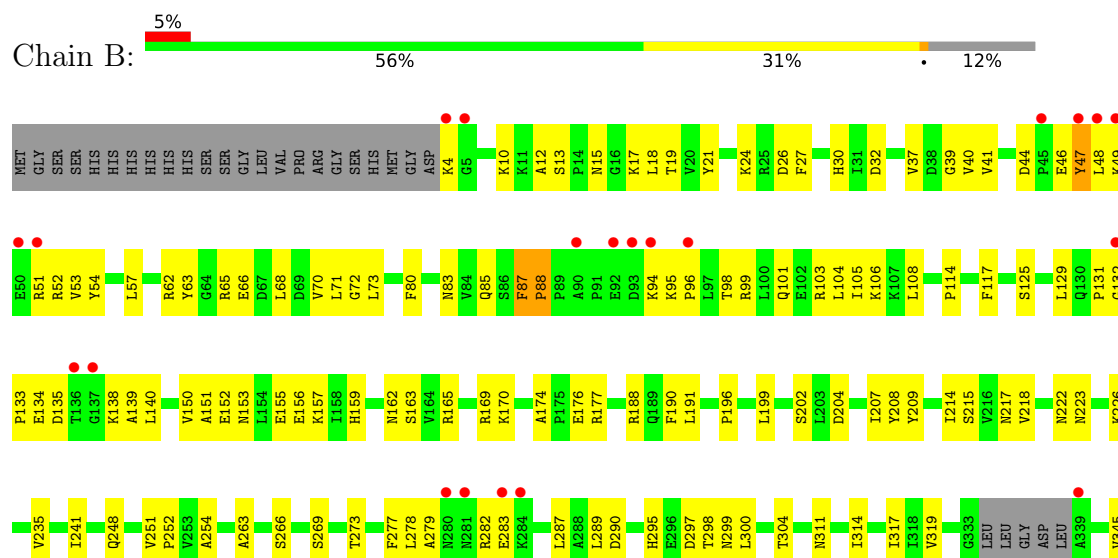
3 Residue-property plots

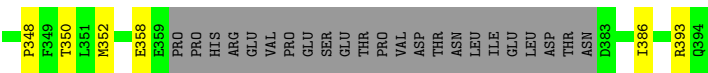
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-arrestin-1

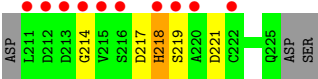


• Molecule 1: Beta-arrestin-1

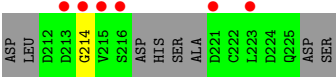




● Molecule 2: peptide from E3 ubiquitin-protein ligase Mdm2



● Molecule 2: peptide from E3 ubiquitin-protein ligase Mdm2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	80.67Å 80.67Å 173.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.34 – 3.00 40.34 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.34-3.00) 100.0 (40.34-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	17.90 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.176 , 0.208 0.174 , 0.204	Depositor DCC
R_{free} test set	1551 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.178 for h,-h-k,-l 0.008 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	1/2940 (0.0%)	0.74	5/3984 (0.1%)
1	B	0.45	0/2926	0.76	0/3970
2	E	0.84	0/109	1.29	1/147 (0.7%)
2	F	0.62	0/70	0.80	0/92
All	All	0.47	1/6045 (0.0%)	0.76	6/8193 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
2	E	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	LYS	C-O	-6.72	1.15	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	TYR	CA-C-N	-6.33	110.89	121.39
1	A	208	TYR	C-N-CA	-6.33	110.89	121.39
2	E	214	GLY	N-CA-C	6.12	127.68	113.18
1	A	66	GLU	CA-C-N	5.90	133.51	121.95
1	A	66	GLU	C-N-CA	5.90	133.51	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	TYR	N-CA-C	5.37	122.10	114.16

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	GLU	Peptide
1	A	283	GLU	Peptide
1	A	46	GLU	Peptide
1	A	71	LEU	Peptide
1	B	15	ASN	Peptide
1	B	152	GLU	Peptide
1	B	47	TYR	Peptide
1	B	87	PHE	Peptide
2	E	218	HIS	Peptide

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	2881	0	2929	107	0
1	B	2867	0	2896	104	0
2	E	109	0	88	11	0
2	F	72	0	55	1	0
3	A	15	0	0	3	0
3	B	10	0	0	0	0
4	A	41	0	0	3	0
4	B	47	0	0	1	0
All	All	6042	0	5968	211	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 18.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HZ1	2:E:221:ASP:HB3	1.24	1.01
1:A:11:LYS:NZ	2:E:221:ASP:HB3	1.76	0.99
1:A:277:PHE:O	1:A:281:ASN:ND2	2.05	0.89
1:A:208:TYR:HB3	1:A:350:THR:O	1.72	0.88
1:B:278:LEU:HD11	1:B:289:LEU:HD22	1.55	0.87
1:A:5:GLY:H	1:A:385:ASP:HB3	1.39	0.87
1:A:254:ALA:HB1	1:A:274:LEU:HD22	1.55	0.86
1:A:176:GLU:HG2	1:A:206:GLU:HB2	1.59	0.83
1:A:226:LYS:HA	1:A:331:ARG:HG2	1.61	0.81
1:A:277:PHE:HB2	1:A:280:ASN:ND2	2.02	0.74
1:B:304:THR:HG23	1:B:319:VAL:H	1.51	0.74
1:A:307:ARG:HE	1:A:310:ALA:HB2	1.52	0.72
1:A:97:LEU:HD23	1:A:102:GLU:HG2	1.70	0.71
1:A:129:LEU:HG	1:A:287:LEU:HA	1.71	0.71
1:A:227:THR:HG22	1:A:264:PRO:HD3	1.71	0.71
1:A:11:LYS:NZ	2:E:221:ASP:CB	2.54	0.69
1:A:275:THR:O	4:A:601:HOH:O	2.10	0.69
1:B:12:ALA:HA	1:B:19:THR:HA	1.75	0.68
1:A:207:ILE:HD11	1:A:214:ILE:HA	1.74	0.68
1:B:263:ALA:O	1:B:266:SER:OG	2.07	0.68
1:B:278:LEU:HB2	1:B:300:LEU:HG	1.74	0.68
1:A:195:LYS:O	4:A:602:HOH:O	2.11	0.68
1:B:159:HIS:HB2	1:B:162:ASN:HB2	1.75	0.68
1:A:15:ASN:HD22	1:A:161:ARG:HB3	1.59	0.66
1:A:225:ASN:HA	1:A:264:PRO:HB3	1.77	0.66
1:B:125:SER:HA	1:B:170:LYS:HE3	1.79	0.65
1:A:228:VAL:HG22	1:A:262:VAL:H	1.61	0.65
1:B:129:LEU:HD13	1:B:241:ILE:HD11	1.80	0.64
1:A:312:ARG:HA	1:A:315:LEU:HD12	1.80	0.64
2:E:217:ASP:OD1	2:E:217:ASP:N	2.31	0.63
1:A:206:GLU:HA	1:A:208:TYR:CE2	2.33	0.63
1:A:277:PHE:HB2	1:A:280:ASN:HD21	1.62	0.63
1:A:250:LYS:NZ	3:A:501:SO4:O2	2.28	0.63
1:A:68:LEU:HD21	2:E:218:HIS:HA	1.80	0.62
1:B:208:TYR:CZ	1:B:214:ILE:HG23	2.35	0.62
1:A:208:TYR:HB2	1:A:351:LEU:HA	1.81	0.62
1:B:37:VAL:HB	1:B:117:PHE:HB2	1.82	0.61
1:A:203:LEU:HD13	1:A:347:LEU:HD22	1.81	0.61
1:B:17:LYS:NZ	1:B:44:ASP:O	2.33	0.61
1:B:10:LYS:HG3	1:B:21:TYR:CE2	2.36	0.61
1:B:222:ASN:ND2	1:B:226:LYS:O	2.28	0.60
1:B:49:LYS:O	1:B:51:ARG:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:OE1	1:A:288:ALA:HB3	2.02	0.59
1:A:18:LEU:HD12	1:A:150:VAL:HG23	1.85	0.58
1:A:25:ARG:NH2	1:A:391:PHE:O	2.34	0.58
1:B:104:LEU:O	1:B:108:LEU:HD13	2.03	0.58
1:B:199:LEU:HD23	1:B:345:VAL:HG13	1.86	0.58
1:B:49:LYS:C	1:B:51:ARG:H	2.11	0.58
1:B:132:GLY:N	1:B:135:ASP:OD1	2.33	0.58
1:A:279:ALA:HA	1:A:282:ARG:CZ	2.35	0.57
1:B:52:ARG:NH1	1:B:85:GLN:OE1	2.37	0.57
1:A:25:ARG:NH2	1:A:392:ALA:O	2.39	0.56
1:A:232:LYS:NZ	1:A:255:MET:SD	2.77	0.56
1:B:30:HIS:O	1:B:32:ASP:N	2.38	0.56
1:A:146:VAL:HG13	1:A:166:LEU:HB2	1.86	0.56
1:B:54:TYR:CE1	1:B:151:ALA:HB3	2.41	0.55
1:B:134:GLU:HG3	1:B:135:ASP:CG	2.31	0.55
1:B:99:ARG:O	1:B:103:ARG:HG3	2.07	0.55
1:A:173:TYR:CE2	1:A:355:LYS:HB2	2.42	0.54
1:A:222:ASN:ND2	1:A:263:ALA:O	2.39	0.54
1:A:99:ARG:H	1:A:99:ARG:HD3	1.73	0.54
1:B:13:SER:N	1:B:18:LEU:O	2.40	0.54
1:B:21:TYR:HB2	1:B:40:VAL:HG12	1.89	0.54
1:B:297:ASP:OD2	1:B:393:ARG:HD3	2.07	0.54
1:B:235:VAL:HB	1:B:254:ALA:HB3	1.89	0.54
1:B:295:HIS:HB2	1:B:298:THR:HG23	1.90	0.54
1:B:98:THR:OG1	1:B:101:GLN:HG3	2.08	0.54
1:A:73:LEU:HD21	1:A:76:ARG:HB2	1.90	0.53
1:B:348:PRO:HB3	4:B:621:HOH:O	2.07	0.53
1:A:48:LEU:CB	1:A:51:ARG:HG3	2.39	0.53
1:B:18:LEU:HD11	1:B:41:VAL:HG13	1.91	0.53
1:B:54:TYR:HE1	1:B:151:ALA:HB3	1.74	0.52
1:B:129:LEU:HD23	1:B:131:PRO:HD3	1.92	0.52
1:A:103:ARG:HH21	1:A:386:ILE:HD11	1.73	0.52
1:A:107:LYS:HD3	1:A:108:LEU:HD22	1.90	0.52
1:A:11:LYS:HZ3	2:E:221:ASP:CG	2.15	0.52
1:A:236:ARG:NH2	3:A:502:SO4:O1	2.37	0.52
1:B:57:LEU:HD23	1:B:80:PHE:HE2	1.75	0.52
1:A:11:LYS:HZ3	2:E:221:ASP:CB	2.22	0.51
1:B:4:LYS:HD2	1:B:103:ARG:HH22	1.74	0.51
1:B:65:ARG:HD2	1:B:71:LEU:O	2.09	0.51
1:B:70:VAL:HG13	1:B:71:LEU:H	1.75	0.51
1:A:63:TYR:HB3	1:A:75:PHE:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HB2	1:A:295:HIS:CD2	2.46	0.51
1:B:153:ASN:HB3	1:B:156:GLU:HB2	1.91	0.51
1:B:278:LEU:HD12	1:B:300:LEU:HG	1.93	0.51
1:A:182:PRO:HD3	1:A:205:LYS:N	2.25	0.51
1:B:24:LYS:HG3	1:B:27:PHE:CE2	2.47	0.50
1:A:11:LYS:NZ	2:E:221:ASP:OD2	2.39	0.50
1:B:174:ALA:HB3	1:B:352:MET:HG3	1.93	0.50
1:B:26:ASP:OD2	1:B:169:ARG:NH1	2.44	0.50
1:A:292:LYS:HB2	1:A:295:HIS:HD2	1.75	0.50
1:A:11:LYS:HB3	1:A:166:LEU:HD21	1.94	0.50
1:A:204:ASP:O	1:A:207:ILE:HB	2.12	0.50
1:B:17:LYS:NZ	1:B:46:GLU:HB2	2.27	0.50
1:B:105:ILE:HD12	1:B:106:LYS:N	2.26	0.49
1:B:358:GLU:HG3	1:B:358:GLU:O	2.13	0.49
1:A:85:GLN:HG2	1:A:88:PRO:HD2	1.95	0.49
1:B:204:ASP:N	1:B:204:ASP:OD1	2.45	0.49
1:B:251:VAL:HG11	1:B:287:LEU:HD13	1.95	0.49
1:A:207:ILE:HD11	1:A:215:SER:H	1.78	0.49
1:B:176:GLU:O	1:B:177:ARG:NH2	2.46	0.49
1:B:153:ASN:OD1	1:B:155:GLU:HG2	2.12	0.49
1:B:174:ALA:O	1:B:209:TYR:OH	2.22	0.49
1:B:44:ASP:O	1:B:46:GLU:N	2.44	0.48
1:A:88:PRO:O	1:A:90:ALA:N	2.47	0.48
1:B:39:GLY:O	1:B:101:GLN:NE2	2.45	0.48
1:B:87:PHE:CD2	1:B:88:PRO:HD3	2.48	0.48
1:B:202:SER:OG	1:B:217:ASN:HB3	2.14	0.48
1:B:62:ARG:NH1	1:B:68:LEU:HD13	2.29	0.48
1:A:214:ILE:N	1:A:274:LEU:O	2.40	0.48
1:A:197:LEU:HD23	1:A:343:VAL:HG21	1.95	0.47
1:A:217:ASN:ND2	1:A:270:LYS:O	2.45	0.47
1:A:87:PHE:O	1:A:89:PRO:HD3	2.14	0.47
1:A:143:ASP:OD1	1:A:143:ASP:N	2.46	0.47
1:B:83:ASN:HD21	2:F:214:GLY:HA3	1.80	0.47
1:A:97:LEU:HD11	1:A:114:PRO:HG3	1.96	0.46
1:A:182:PRO:HD3	1:A:205:LYS:CA	2.44	0.46
1:A:159:HIS:HB3	1:A:161:ARG:NH2	2.30	0.46
1:A:285:ARG:HB3	1:A:287:LEU:HD11	1.98	0.46
1:B:53:VAL:HG12	1:B:87:PHE:HB2	1.97	0.46
1:B:4:LYS:HB2	1:B:4:LYS:HE2	1.72	0.46
1:B:66:GLU:HA	1:B:66:GLU:OE2	2.15	0.46
1:A:198:HIS:HB3	1:A:221:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:HD2	1:B:72:GLY:HA3	1.98	0.46
1:A:56:THR:O	1:A:146:VAL:HA	2.16	0.46
1:B:157:LYS:HA	1:B:157:LYS:HD3	1.73	0.46
1:A:29:ASP:OD2	4:A:603:HOH:O	2.20	0.45
1:B:196:PRO:HD2	1:B:223:ASN:HB2	1.98	0.45
1:A:128:THR:OG1	1:A:291:GLY:O	2.32	0.45
1:B:138:LYS:HG3	1:B:139:ALA:H	1.82	0.45
1:B:70:VAL:HG13	1:B:71:LEU:N	2.31	0.45
1:B:104:LEU:HD12	1:B:108:LEU:HD11	1.98	0.45
1:B:278:LEU:HD23	1:B:278:LEU:O	2.16	0.45
1:A:15:ASN:OD1	1:A:17:LYS:HG2	2.16	0.45
1:B:47:TYR:CG	1:B:48:LEU:N	2.85	0.45
1:B:138:LYS:HD3	1:B:138:LYS:HA	1.73	0.45
1:B:215:SER:HG	1:B:273:THR:HG1	1.64	0.45
1:A:39:GLY:HA3	1:A:115:PHE:CZ	2.52	0.45
1:A:68:LEU:HB3	2:E:219:SER:O	2.17	0.45
1:A:11:LYS:HD3	1:A:166:LEU:CD2	2.47	0.45
1:B:49:LYS:C	1:B:51:ARG:N	2.76	0.44
1:B:290:ASP:OD2	1:B:299:ASN:ND2	2.43	0.44
1:B:68:LEU:HD23	1:B:165:ARG:NH1	2.33	0.44
1:B:277:PHE:O	1:B:278:LEU:HB3	2.17	0.44
1:B:51:ARG:C	1:B:52:ARG:HG3	2.42	0.44
1:B:85:GLN:HG2	1:B:87:PHE:O	2.16	0.44
1:A:238:TYR:CE1	1:A:322:LYS:HE3	2.52	0.44
1:A:292:LYS:O	1:A:298:THR:OG1	2.34	0.44
1:A:208:TYR:CB	1:A:351:LEU:HA	2.46	0.44
1:A:289:LEU:HD11	1:A:293:LEU:HD13	2.00	0.44
1:B:278:LEU:HD11	1:B:289:LEU:CD2	2.38	0.44
1:A:199:LEU:HB2	1:A:327:LEU:HD11	1.99	0.44
1:A:214:ILE:O	1:A:273:THR:HA	2.18	0.44
1:A:229:LYS:CE	1:A:330:SER:HB3	2.48	0.44
1:A:131:PRO:HG2	1:A:137:GLY:C	2.43	0.43
1:B:218:VAL:O	1:B:269:SER:HA	2.18	0.43
1:B:241:ILE:HD13	1:B:317:ILE:HG23	1.99	0.43
1:B:150:VAL:HG22	1:B:162:ASN:HB3	2.01	0.43
1:A:235:VAL:HB	1:A:254:ALA:HB3	2.00	0.43
1:B:12:ALA:HB1	1:B:19:THR:HG22	2.00	0.43
1:A:207:ILE:HG23	1:A:207:ILE:O	2.18	0.43
1:A:250:LYS:NZ	3:A:501:SO4:S	2.91	0.43
1:B:282:ARG:O	1:B:283:GLU:HG3	2.18	0.43
1:A:272:TYR:CD1	1:A:272:TYR:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:HD22	2:E:219:SER:N	2.33	0.43
1:A:102:GLU:HA	1:A:105:ILE:HG12	1.99	0.43
1:B:207:ILE:HD13	1:B:350:THR:HB	2.00	0.43
1:B:304:THR:CG2	1:B:319:VAL:H	2.25	0.43
1:A:14:PRO:HG2	1:A:160:LYS:O	2.18	0.43
1:A:45:PRO:HD2	1:A:111:HIS:CE1	2.54	0.43
1:B:95:LYS:O	1:B:95:LYS:HG2	2.18	0.43
1:A:204:ASP:O	1:A:206:GLU:N	2.52	0.43
1:B:188:ARG:HG2	1:B:190:PHE:CZ	2.54	0.42
1:A:201:ALA:HA	1:A:217:ASN:O	2.19	0.42
1:A:30:HIS:O	1:A:31:ILE:C	2.62	0.42
1:A:181:GLN:HB3	1:A:203:LEU:O	2.19	0.42
1:A:230:LYS:HD2	1:A:257:GLU:CD	2.45	0.42
1:B:108:LEU:HD12	1:B:108:LEU:N	2.34	0.42
1:B:277:PHE:C	1:B:279:ALA:H	2.28	0.42
1:A:25:ARG:HH21	1:A:391:PHE:C	2.26	0.42
1:A:321:TYR:HB3	1:A:349:PHE:CZ	2.54	0.42
1:B:94:LYS:HA	1:B:96:PRO:HD2	2.02	0.42
1:B:132:GLY:HA3	1:B:133:PRO:HD2	1.89	0.42
1:B:235:VAL:O	1:B:252:PRO:HA	2.19	0.42
1:B:287:LEU:HD21	1:B:300:LEU:HD21	2.02	0.42
1:A:53:VAL:HG12	1:A:87:PHE:CB	2.50	0.42
1:A:228:VAL:HA	1:A:328:VAL:O	2.19	0.42
1:B:40:VAL:HA	1:B:114:PRO:HA	2.01	0.42
1:A:51:ARG:NE	1:A:152:GLU:OE2	2.52	0.41
1:A:13:SER:HB2	1:A:161:ARG:O	2.20	0.41
1:A:76:ARG:HG2	1:B:188:ARG:HD2	2.01	0.41
1:A:207:ILE:CD1	1:A:214:ILE:HA	2.45	0.41
1:B:104:LEU:HD13	1:B:386:ILE:HD13	2.02	0.41
1:B:159:HIS:O	1:B:163:SER:OG	2.35	0.41
1:B:350:THR:HG22	1:B:352:MET:HG2	2.03	0.41
1:A:279:ALA:C	1:A:281:ASN:H	2.28	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.86	0.41
1:B:248:GLN:CD	1:B:248:GLN:N	2.78	0.41
1:A:90:ALA:O	1:A:92:GLU:HG3	2.20	0.41
1:B:290:ASP:C	1:B:290:ASP:OD1	2.64	0.41
1:A:25:ARG:HH21	1:A:392:ALA:C	2.28	0.41
1:B:62:ARG:HB3	1:B:73:LEU:HD11	2.03	0.41
1:A:11:LYS:NZ	2:E:221:ASP:CG	2.78	0.40
1:A:129:LEU:HD23	1:A:130:GLN:N	2.35	0.40
1:A:24:LYS:HE3	1:A:24:LYS:HB2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ALA:CB	1:B:19:THR:HG22	2.51	0.40
1:B:63:TYR:CE2	1:B:140:LEU:HD22	2.56	0.40
1:B:95:LYS:O	1:B:96:PRO:C	2.64	0.40
1:A:99:ARG:HD3	1:A:99:ARG:N	2.35	0.40
1:B:311:ASN:OD1	1:B:314:ILE:HG23	2.21	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	357/414 (86%)	330 (92%)	27 (8%)	0	100	100
1	B	357/414 (86%)	334 (94%)	22 (6%)	1 (0%)	36	70
2	E	13/18 (72%)	7 (54%)	6 (46%)	0	100	100
2	F	6/18 (33%)	5 (83%)	1 (17%)	0	100	100
All	All	733/864 (85%)	676 (92%)	56 (8%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/368 (87%)	319 (100%)	1 (0%)	86	91
1	B	318/368 (86%)	318 (100%)	0	100	100
2	E	13/16 (81%)	13 (100%)	0	100	100
2	F	9/16 (56%)	9 (100%)	0	100	100
All	All	660/768 (86%)	659 (100%)	1 (0%)	87	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	217	ASN
1	A	280	ASN
1	B	172	GLN
1	B	281	ASN
1	B	353	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands 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	$\# Z > 2$
3	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.30	0
3	SO4	B	502	-	4,4,4	0.35	0	6,6,6	0.41	0
3	SO4	A	501	-	4,4,4	0.35	0	6,6,6	0.18	0
3	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.19	0
3	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.16	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	SO4	1	0
3	A	501	SO4	2	0

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, 95th 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	363/414 (87%)	0.01	20 (5%) 30 15	2, 17, 60, 103	0
1	B	363/414 (87%)	0.03	21 (5%) 29 15	2, 15, 63, 93	0
2	E	15/18 (83%)	2.20	10 (66%) 0 0	45, 57, 68, 71	0
2	F	10/18 (55%)	2.06	6 (60%) 0 0	36, 55, 58, 61	0
All	All	751/864 (86%)	0.09	57 (7%) 20 10	2, 18, 64, 103	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ARG	7.8
1	A	135	ASP	7.5
1	A	133	PRO	6.2
1	B	48	LEU	5.4
1	A	136	THR	4.9
1	B	94	LYS	4.8
2	E	219	SER	4.2
1	B	50	GLU	3.9
1	B	136	THR	3.9
2	E	215	VAL	3.9
1	B	5	GLY	3.8
1	A	137	GLY	3.8
1	B	92	GLU	3.7
1	A	46	GLU	3.6
1	B	47	TYR	3.6
1	A	132	GLY	3.6
1	B	45	PRO	3.5
1	B	283	GLU	3.4
2	F	216	SER	3.4
2	E	214	GLY	3.3
1	B	93	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	69	ASP	3.3
2	F	213	ASP	3.3
2	E	222	CYS	3.1
1	A	50	GLU	3.1
1	A	131	PRO	3.0
1	B	280	ASN	3.0
1	A	134	GLU	2.9
2	F	223	LEU	2.8
2	E	212	ASP	2.7
2	E	213	ASP	2.6
1	A	204	ASP	2.6
1	A	48	LEU	2.5
1	B	49	LYS	2.5
1	B	339	ALA	2.5
2	E	218	HIS	2.5
1	B	284	LYS	2.5
1	B	137	GLY	2.4
1	B	132	GLY	2.4
1	B	4	LYS	2.4
1	A	47	TYR	2.4
1	A	206	GLU	2.3
1	A	333	GLY	2.3
1	B	90	ALA	2.3
2	F	214	GLY	2.2
1	A	208	TYR	2.2
2	E	216	SER	2.2
2	E	211	LEU	2.2
1	B	281	ASN	2.2
2	F	221	ASP	2.2
1	A	11	LYS	2.1
2	E	220	ALA	2.1
1	A	5	GLY	2.1
1	A	49	LYS	2.0
1	B	96	PRO	2.0
2	F	215	VAL	2.0
1	A	71	LEU	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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, 95th 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	501	5/5	0.75	0.24	61,63,73,95	0
3	SO4	B	501	5/5	0.89	0.15	68,68,78,95	0
3	SO4	A	503	5/5	0.94	0.19	44,57,62,80	0
3	SO4	B	502	5/5	0.94	0.14	31,44,48,58	0
3	SO4	A	502	5/5	0.96	0.13	27,35,37,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.