



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 05:00 PM EDT

PDB ID : 5IJ8
Title : Structure of the primary oncogenic mutant Y641N Hs/AcPRC2 in complex with a pyridone inhibitor
Authors : Gajiwala, K.S.; Brooun, A.; Deng, Y.-L.; Liu, W.
Deposited on : 2016-03-01
Resolution : 2.99 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

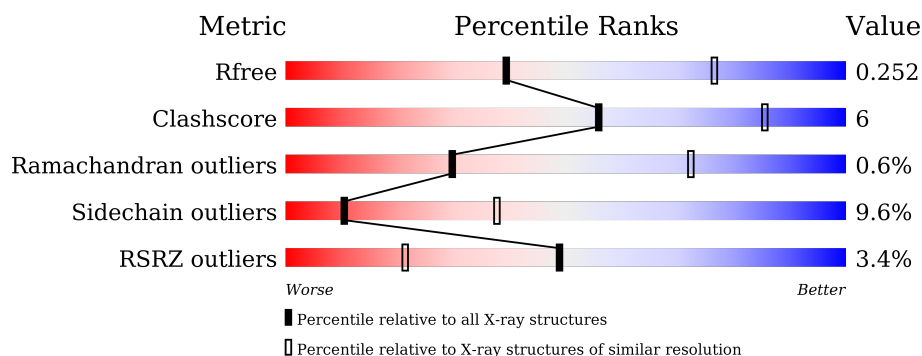
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	643	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>13%</div> <div>•</div> <div>28%</div> </div> </div>
1	B	643	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>13%</div> <div>•</div> <div>28%</div> </div> </div>
2	E	362	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>••</div> </div> </div>
2	F	362	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>
3	S	191	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>16%</div> <div>•</div> <div>33%</div> </div> </div>
3	T	191	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>15%</div> <div>•</div> <div>33%</div> </div> </div>

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
5	ZN	A	9005	-	-	-	X
5	ZN	B	9007	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15580 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 Enhancer of Zeste Homolog 2 (EZH2), Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3771	2363	680	689	39			
1	B	466	Total	C	N	O	S	0	0	0
			3779	2366	681	693	39			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q15910
A	?	-	PRO	deletion	UNP Q15910
A	?	-	ARG	deletion	UNP Q15910
A	?	-	LYS	deletion	UNP Q15910
A	492	LEU	LYS	linker	UNP Q15910
A	493	GLY	LYS	linker	UNP Q15910
A	494	GLY	ARG	linker	UNP Q15910
A	495	GLY	LYS	linker	UNP Q15910
A	496	GLY	HIS	linker	UNP Q15910
A	497	SER	ARG	linker	UNP Q15910
A	498	GLY	LEU	linker	UNP Q15910
A	499	GLY	TRP	linker	UNP Q15910
A	500	GLY	ALA	linker	UNP Q15910
A	501	GLY	ALA	linker	UNP Q15910
A	502	SER	HIS	linker	UNP Q15910
A	503	GLY	CYS	linker	UNP Q15910
A	504	GLY	ARG	linker	UNP Q15910
A	505	GLY	LYS	linker	UNP Q15910
A	506	GLY	ILE	linker	UNP Q15910
A	507	SER	GLN	linker	UNP Q15910
A	508	ALA	LEU	linker	UNP Q15910
A	509	ALA	LYS	linker	UNP Q15910
A	510	ALA	LYS	linker	UNP Q15910
A	532	ASN	SER	linker	UNP Q15910

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Chain	Residue	Modelled	Actual	Comment	Reference
A	641	ASN	TYR	engineered mutation	UNP Q15910
B	?	-	PRO	deletion	UNP Q15910
B	?	-	PRO	deletion	UNP Q15910
B	?	-	ARG	deletion	UNP Q15910
B	?	-	LYS	deletion	UNP Q15910
B	492	LEU	LYS	linker	UNP Q15910
B	493	GLY	LYS	linker	UNP Q15910
B	494	GLY	ARG	linker	UNP Q15910
B	495	GLY	LYS	linker	UNP Q15910
B	496	GLY	HIS	linker	UNP Q15910
B	497	SER	ARG	linker	UNP Q15910
B	498	GLY	LEU	linker	UNP Q15910
B	499	GLY	TRP	linker	UNP Q15910
B	500	GLY	ALA	linker	UNP Q15910
B	501	GLY	ALA	linker	UNP Q15910
B	502	SER	HIS	linker	UNP Q15910
B	503	GLY	CYS	linker	UNP Q15910
B	504	GLY	ARG	linker	UNP Q15910
B	505	GLY	LYS	linker	UNP Q15910
B	506	GLY	ILE	linker	UNP Q15910
B	507	SER	GLN	linker	UNP Q15910
B	508	ALA	LEU	linker	UNP Q15910
B	509	ALA	LYS	linker	UNP Q15910
B	510	ALA	LYS	linker	UNP Q15910
B	532	ASN	SER	linker	UNP Q15910
B	641	ASN	TYR	engineered mutation	UNP Q15910

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	358	Total	C	N	O	S	0	0	0
			2898	1834	509	534	21			
2	F	359	Total	C	N	O	S	0	0	0
			2906	1840	510	535	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	66	MET	-	initiating methionine	UNP O75530
F	66	MET	-	initiating methionine	UNP O75530

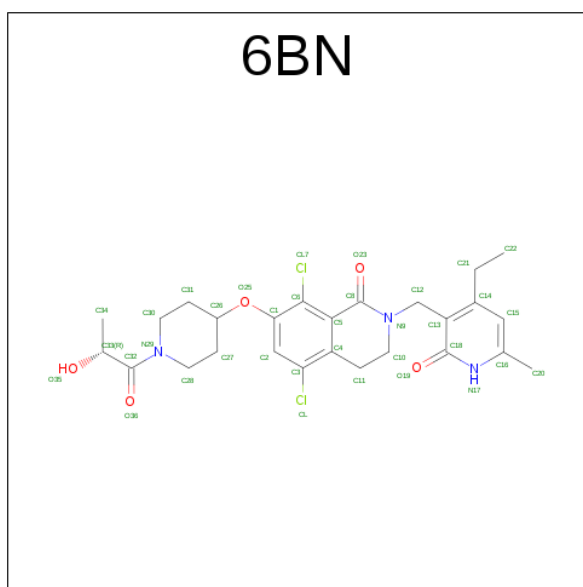
- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			
3	T	128	Total	C	N	O	S	0	0	0
			1070	675	185	198	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	535	MET	-	initiating methionine	UNP Q15022
S	536	ASP	-	expression tag	UNP Q15022
S	537	TYR	-	expression tag	UNP Q15022
S	538	LYS	-	expression tag	UNP Q15022
S	539	ASP	-	expression tag	UNP Q15022
S	540	ASP	-	expression tag	UNP Q15022
S	541	ASP	-	expression tag	UNP Q15022
S	542	ASP	-	expression tag	UNP Q15022
S	543	LYS	-	expression tag	UNP Q15022
S	544	GLY	-	expression tag	UNP Q15022
S	583	ASP	SER	engineered mutation	UNP Q15022
T	535	MET	-	initiating methionine	UNP Q15022
T	536	ASP	-	expression tag	UNP Q15022
T	537	TYR	-	expression tag	UNP Q15022
T	538	LYS	-	expression tag	UNP Q15022
T	539	ASP	-	expression tag	UNP Q15022
T	540	ASP	-	expression tag	UNP Q15022
T	541	ASP	-	expression tag	UNP Q15022
T	542	ASP	-	expression tag	UNP Q15022
T	543	LYS	-	expression tag	UNP Q15022
T	544	GLY	-	expression tag	UNP Q15022
T	583	ASP	SER	engineered mutation	UNP Q15022

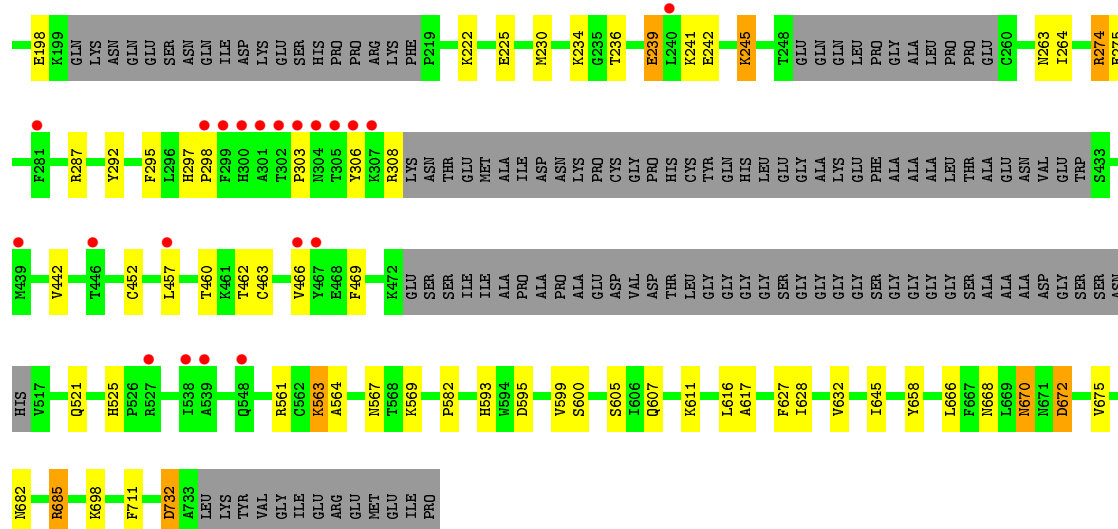
- Molecule 4 is 5,8-dichloro-2-[(4-ethyl-6-methyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-7-({1-[(2R)-2-hydroxypropanoyl]piperidin-4-yl}oxy)-3,4-dihydroisoquinolin-1(2H)-one (three-letter code: 6BN) (formula: C₂₆H₃₁Cl₂N₃O₅).



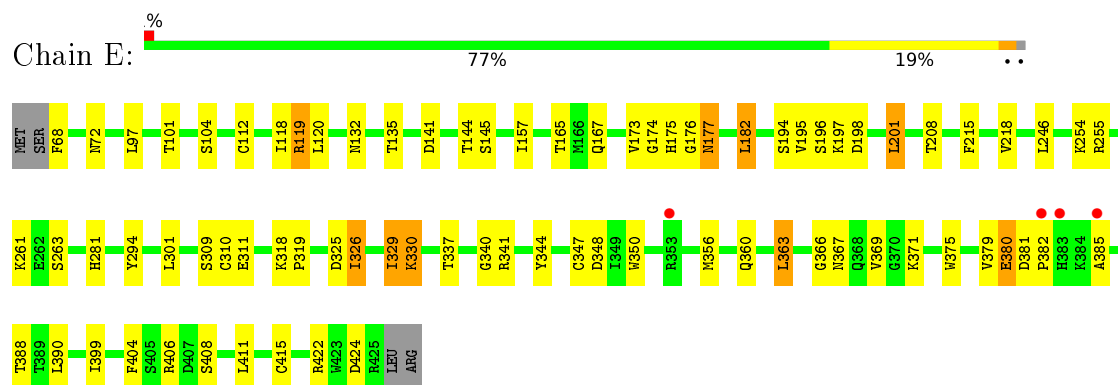
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 36	C 26	Cl 2	N 3	O 5	0	0
4	B	1	Total 36	C 26	Cl 2	N 3	O 5	0	0

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

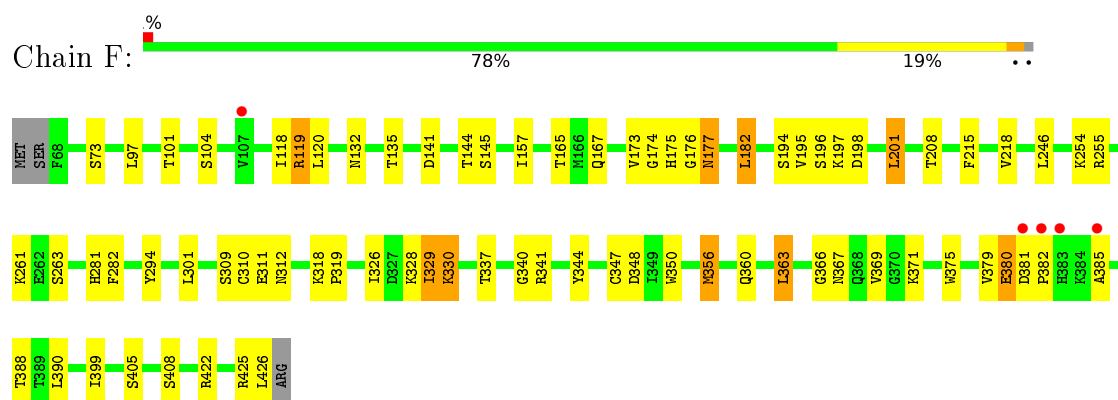
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	7	Total Zn 7 7	0	0
5	A	7	Total Zn 7 7	0	0



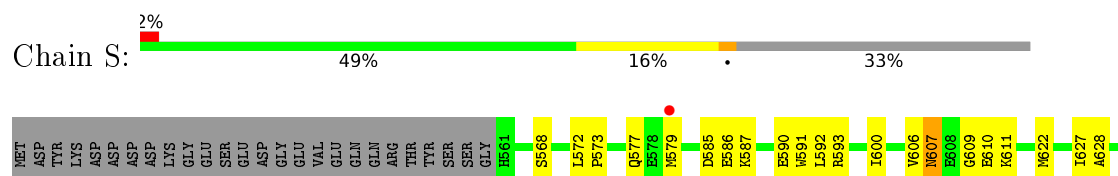
• Molecule 2: Polycomb protein EED

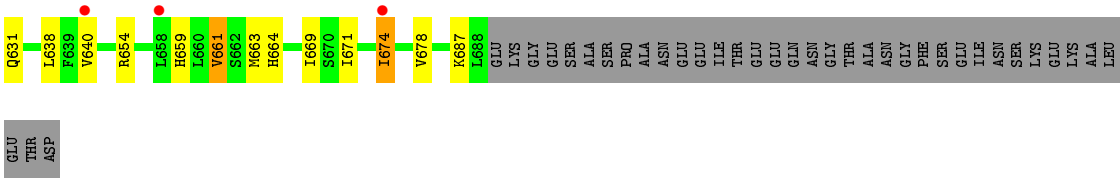


• Molecule 2: Polycomb protein EED

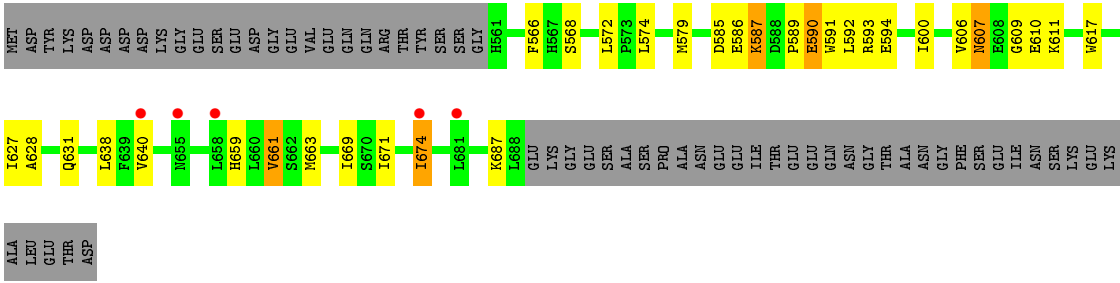


• Molecule 3: Polycomb protein SUZ12





● Molecule 3: Polycomb protein SUZ12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 115.13Å 153.94Å 90.00° 103.35° 90.00°	Depositor
Resolution (Å)	91.28 – 2.99 91.28 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.28-2.99) 99.7 (91.28-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.188 , 0.240 0.198 , 0.252	Depositor DCC
R_{free} test set	2491 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15580	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 6BN

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	0.52	0/3851	0.72	0/5177
1	B	0.52	0/3857	0.71	0/5185
2	E	0.50	0/2972	0.73	0/4026
2	F	0.50	0/2980	0.75	1/4037 (0.0%)
3	S	0.51	0/1091	0.71	0/1464
3	T	0.51	0/1091	0.71	0/1464
All	All	0.51	0/15842	0.72	1/21353 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	356	MET	C-N-CA	5.08	134.40	121.70

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	3771	0	3661	39	0
1	B	3779	0	3674	48	0
2	E	2898	0	2812	45	0
2	F	2906	0	2823	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	S	1070	0	1052	23	0
3	T	1070	0	1052	25	0
4	A	36	0	0	0	0
4	B	36	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
All	All	15580	0	15074	187	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 6.

All (187) 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)
3:S:628:ALA:H	3:S:631:GLN:HE21	1.26	0.83
3:T:628:ALA:H	3:T:631:GLN:HE21	1.26	0.82
1:B:670:ASN:HD22	1:B:672:ASP:H	1.28	0.79
3:T:627:ILE:H	3:T:631:GLN:NE2	1.81	0.79
3:T:606:VAL:HG13	3:T:610:GLU:HG3	1.65	0.78
2:F:330:LYS:H	2:F:330:LYS:HE2	1.48	0.78
2:E:330:LYS:H	2:E:330:LYS:HE2	1.48	0.77
3:S:627:ILE:H	3:S:631:GLN:NE2	1.81	0.77
1:B:57:ASN:HD22	2:E:406:ARG:HH21	1.33	0.75
1:B:263:ASN:HB3	3:S:607:ASN:ND2	2.02	0.74
3:T:607:ASN:HD22	3:T:609:GLY:H	1.34	0.73
2:E:379:VAL:HG21	2:E:385:ALA:HA	1.71	0.73
1:A:452:CYS:HG	1:A:463:CYS:HG	1.27	0.73
2:F:379:VAL:HG21	2:F:385:ALA:HA	1.69	0.72
1:A:106:SER:HB3	2:F:157:ILE:HD11	1.73	0.71
2:E:201:LEU:HB2	2:E:215:PHE:HB2	1.74	0.70
3:S:607:ASN:HD22	3:S:609:GLY:H	1.36	0.70
2:E:294:TYR:CZ	2:E:350:TRP:HB3	2.27	0.69
2:F:294:TYR:OH	2:F:310:CYS:HB3	1.93	0.69
2:F:201:LEU:HB2	2:F:215:PHE:HB2	1.75	0.68
3:S:661:VAL:HA	3:S:674:ILE:HD11	1.76	0.68
3:T:663:MET:HB3	3:T:669:ILE:HG12	1.76	0.68
2:E:294:TYR:OH	2:E:310:CYS:HB3	1.93	0.68
2:F:294:TYR:CZ	2:F:350:TRP:HB3	2.29	0.67
1:B:94:GLN:HE22	2:E:119:ARG:HA	1.56	0.67
3:S:663:MET:HB3	3:S:669:ILE:HG12	1.75	0.67
3:T:661:VAL:HA	3:T:674:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HD13	1:A:97:PRO:HD2	1.77	0.67
1:B:96:ILE:HD13	1:B:97:PRO:HD2	1.75	0.67
1:B:110:MET:O	2:E:176:GLY:HA3	1.95	0.66
1:A:263:ASN:HB3	3:T:607:ASN:ND2	2.10	0.66
1:A:292:TYR:OH	3:T:659:HIS:HD2	1.80	0.65
3:S:628:ALA:HB3	3:S:631:GLN:HG3	1.80	0.63
3:T:628:ALA:HB3	3:T:631:GLN:HG3	1.80	0.63
2:E:165:THR:HG22	2:E:167:GLN:HG2	1.80	0.63
2:E:319:PRO:HB2	2:E:329:ILE:HD13	1.81	0.63
1:B:292:TYR:OH	3:S:659:HIS:HD2	1.83	0.62
2:E:175:HIS:HE1	2:E:194:SER:OG	1.82	0.61
3:S:627:ILE:H	3:S:631:GLN:HE22	1.48	0.61
1:B:682:ASN:O	1:B:685:ARG:HG2	2.01	0.61
3:T:627:ILE:H	3:T:631:GLN:HE22	1.49	0.61
1:A:682:ASN:O	1:A:685:ARG:HG2	2.01	0.60
1:B:106:SER:HB3	2:E:157:ILE:HD11	1.83	0.60
1:A:670:ASN:ND2	1:A:672:ASP:H	2.00	0.59
1:B:71:MET:CE	1:B:99:LYS:HB2	2.32	0.59
2:F:319:PRO:HB2	2:F:329:ILE:HD13	1.82	0.59
2:F:165:THR:HG22	2:F:167:GLN:HG2	1.84	0.59
3:S:606:VAL:HG13	3:S:610:GLU:HG3	1.86	0.57
1:B:242:GLU:HA	1:B:245:LYS:HB2	1.87	0.57
1:B:599:VAL:HG12	1:B:600:SER:H	1.70	0.57
1:A:582:PRO:HD3	1:A:607:GLN:HE22	1.70	0.57
1:A:599:VAL:HG12	1:A:600:SER:H	1.69	0.56
1:B:582:PRO:HD3	1:B:607:GLN:HE22	1.70	0.56
1:B:670:ASN:ND2	1:B:672:ASP:H	2.01	0.56
1:B:57:ASN:HD22	2:E:406:ARG:NH2	2.00	0.56
2:F:195:VAL:HG22	2:F:201:LEU:HD13	1.87	0.56
1:B:274:ARG:HB2	1:B:442:VAL:HA	1.87	0.55
1:B:71:MET:HE1	1:B:99:LYS:HB2	1.89	0.55
1:A:110:MET:O	2:F:176:GLY:HA3	2.06	0.55
2:E:195:VAL:HG22	2:E:201:LEU:HD13	1.87	0.55
2:F:97:LEU:HD13	2:F:405:SER:HB2	1.88	0.55
1:B:85:VAL:HG23	2:E:120:LEU:HD22	1.90	0.54
2:E:366:GLY:HA3	2:E:399:ILE:HB	1.91	0.53
1:B:222:LYS:HA	1:B:225:GLU:HG2	1.90	0.53
3:S:606:VAL:HG12	3:S:611:LYS:HG3	1.91	0.53
2:F:157:ILE:HG12	2:F:173:VAL:HG22	1.91	0.53
2:E:157:ILE:HG12	2:E:173:VAL:HG22	1.92	0.52
2:F:218:VAL:HG22	2:F:281:HIS:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:LYS:HB3	1:B:711:PHE:HE2	1.75	0.51
2:F:366:GLY:HA3	2:F:399:ILE:HB	1.92	0.51
3:T:607:ASN:ND2	3:T:609:GLY:H	2.07	0.51
3:T:589:PRO:HG2	3:T:592:LEU:HD12	1.92	0.51
1:A:94:GLN:HE22	2:F:119:ARG:HA	1.76	0.51
1:A:698:LYS:HB3	1:A:711:PHE:HE2	1.75	0.50
1:B:563:LYS:HE2	1:B:564:ALA:H	1.77	0.50
3:S:607:ASN:ND2	3:S:610:GLU:H	2.09	0.50
2:E:218:VAL:HG22	2:E:281:HIS:HB3	1.93	0.49
1:B:616:LEU:HD22	3:S:568:SER:HA	1.94	0.49
1:A:117:GLN:HG2	3:T:587:LYS:HA	1.94	0.49
1:A:563:LYS:HE2	1:A:564:ALA:H	1.77	0.49
2:E:301:LEU:HA	2:E:360:GLN:HE22	1.77	0.49
1:A:698:LYS:HB3	1:A:711:PHE:CE2	2.47	0.49
1:B:658:TYR:HD2	1:B:666:LEU:HD21	1.78	0.49
2:E:68:PHE:HA	2:E:424:ASP:O	2.13	0.49
1:A:303:PRO:HA	1:A:306:TYR:CZ	2.48	0.49
3:T:607:ASN:ND2	3:T:610:GLU:H	2.11	0.49
1:B:698:LYS:HB3	1:B:711:PHE:CE2	2.48	0.48
2:F:301:LEU:HA	2:F:360:GLN:NE2	2.29	0.48
2:E:301:LEU:HA	2:E:360:GLN:NE2	2.28	0.48
1:A:28:GLN:HE21	1:A:28:GLN:HA	1.78	0.48
2:F:340:GLY:HA3	2:F:382:PRO:HG2	1.96	0.48
2:F:301:LEU:HA	2:F:360:GLN:HE22	1.79	0.48
1:A:658:TYR:HD2	1:A:666:LEU:HD21	1.79	0.47
1:B:303:PRO:HA	1:B:306:TYR:CZ	2.49	0.47
1:A:566:CYS:SG	1:A:571:CYS:SG	3.11	0.47
1:A:172:VAL:HG13	1:A:244:TYR:HE1	1.79	0.47
2:E:340:GLY:HA3	2:E:382:PRO:HG2	1.97	0.47
2:E:177:ASN:HB3	2:E:197:LYS:HB3	1.96	0.47
3:S:607:ASN:HD22	3:S:609:GLY:N	2.09	0.47
1:A:85:VAL:HG23	2:F:120:LEU:HD22	1.95	0.47
3:T:590:GLU:O	3:T:593:ARG:HB2	2.14	0.47
1:A:82:GLU:HG2	1:A:97:PRO:HA	1.97	0.47
2:F:208:THR:HG21	2:F:263:SER:O	2.15	0.47
3:T:606:VAL:HG12	3:T:611:LYS:HG3	1.97	0.47
1:B:563:LYS:HD3	1:B:563:LYS:H	1.80	0.46
1:B:668:ASN:HD22	1:B:732:ASP:HB3	1.80	0.46
2:F:135:THR:HG23	2:F:182:LEU:HD22	1.97	0.46
2:F:309:SER:HB3	2:F:311:GLU:HG2	1.97	0.46
2:E:135:THR:HG23	2:E:182:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HG12	3:S:654:ARG:HB3	1.97	0.46
1:B:599:VAL:HG12	1:B:600:SER:N	2.31	0.46
2:E:208:THR:HG21	2:E:263:SER:O	2.15	0.46
3:T:607:ASN:HD22	3:T:609:GLY:N	2.08	0.46
1:A:616:LEU:HD22	3:T:568:SER:HA	1.98	0.46
1:A:560:CYS:SG	1:A:566:CYS:SG	3.13	0.46
2:F:141:ASP:HB3	2:F:144:THR:HB	1.98	0.46
2:F:196:SER:HB3	2:F:198:ASP:OD1	2.15	0.46
2:E:309:SER:HB3	2:E:311:GLU:HG2	1.99	0.45
3:S:607:ASN:ND2	3:S:609:GLY:H	2.07	0.45
2:E:141:ASP:HB3	2:E:144:THR:HB	1.99	0.45
2:F:218:VAL:HG11	3:T:591:TRP:CE3	2.51	0.45
1:B:52:ARG:HA	1:B:55:ILE:HD12	1.99	0.45
1:A:297:HIS:HA	1:A:298:PRO:HD3	1.86	0.44
1:A:599:VAL:HG12	1:A:600:SER:N	2.32	0.44
1:B:617:ALA:HB3	1:B:627:PHE:CE2	2.52	0.44
1:B:308:ARG:HH21	3:S:664:HIS:CE1	2.36	0.44
1:B:94:GLN:NE2	2:E:120:LEU:H	2.16	0.44
1:B:57:ASN:ND2	2:E:406:ARG:HH21	2.08	0.44
1:A:563:LYS:HD3	1:A:563:LYS:H	1.81	0.44
2:F:177:ASN:HB3	2:F:197:LYS:HB3	2.00	0.44
2:F:344:TYR:HE1	2:F:347:CYS:HB3	1.83	0.43
2:E:196:SER:HB3	2:E:198:ASP:OD1	2.17	0.43
2:E:344:TYR:HE1	2:E:347:CYS:HB3	1.83	0.43
1:A:89:LEU:HD13	2:F:73:SER:HB3	2.01	0.43
2:E:404:PHE:CE1	2:E:411:LEU:HD13	2.54	0.43
1:A:119:ASN:HB3	1:A:645:ILE:HG12	2.00	0.43
2:E:104:SER:O	2:E:132:ASN:HA	2.18	0.43
2:F:282:PHE:CE2	3:T:594:GLU:HB3	2.54	0.43
1:A:444:ILE:HG22	1:A:454:ILE:HD13	2.00	0.43
2:F:104:SER:O	2:F:132:ASN:HA	2.19	0.43
1:B:171:PHE:O	1:B:175:VAL:HG23	2.19	0.42
1:A:670:ASN:HD22	1:A:672:ASP:H	1.67	0.42
1:B:119:ASN:HB3	1:B:645:ILE:HG12	2.00	0.42
1:A:16:ARG:HD2	1:A:230:MET:HE2	2.01	0.42
2:E:367:ASN:HB2	2:E:371:LYS:H	1.85	0.42
2:E:218:VAL:HG11	3:S:591:TRP:CE3	2.54	0.42
1:A:617:ALA:HB3	1:A:627:PHE:CE2	2.54	0.42
2:F:363:LEU:HD23	2:F:375:TRP:CE3	2.55	0.42
3:S:600:ILE:HG22	3:S:611:LYS:HG2	2.01	0.42
2:E:330:LYS:CE	2:E:330:LYS:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:LYS:HG2	2:E:337:THR:HB	2.01	0.42
2:E:97:LEU:HB2	2:E:112:CYS:HB2	2.02	0.42
1:A:236:THR:HG23	1:A:239:GLU:H	1.85	0.42
1:B:263:ASN:HB3	3:S:607:ASN:HD21	1.82	0.42
1:B:297:HIS:HA	1:B:298:PRO:HD3	1.87	0.42
1:B:295:PHE:CE2	3:S:592:LEU:HD22	2.55	0.42
1:B:236:THR:HG23	1:B:239:GLU:H	1.84	0.42
2:E:165:THR:HG22	2:E:167:GLN:CG	2.50	0.42
2:F:318:LYS:HG2	2:F:337:THR:HB	2.02	0.42
3:T:590:GLU:HB3	3:T:593:ARG:NH2	2.34	0.42
2:F:118:ILE:HD11	2:F:422:ARG:HB2	2.02	0.42
2:F:312:ASN:HA	2:F:344:TYR:CE1	2.56	0.41
3:T:590:GLU:HG3	3:T:590:GLU:H	1.70	0.41
1:B:16:ARG:HD2	1:B:230:MET:CE	2.50	0.41
2:F:367:ASN:HB3	2:F:369:VAL:H	1.85	0.41
1:B:116:LEU:HA	1:B:116:LEU:HD12	1.91	0.41
1:B:166:ILE:HG23	1:B:234:LYS:HD3	2.02	0.41
2:F:367:ASN:HB2	2:F:371:LYS:H	1.85	0.41
1:B:83:CYS:HB3	1:B:98:LEU:HG	2.01	0.41
2:F:175:HIS:HE1	2:F:194:SER:OG	2.02	0.41
3:S:593:ARG:HG2	3:S:622:MET:HE2	2.03	0.41
1:A:461:LYS:HD3	1:A:461:LYS:HA	1.92	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.90	0.41
1:A:432:TRP:CE2	1:A:461:LYS:HD2	2.56	0.41
3:T:617:TRP:CZ2	3:T:663:MET:HE1	2.56	0.41
2:E:68:PHE:HB2	2:E:390:LEU:HD11	2.03	0.40
1:A:618:PRO:HD3	3:T:566:PHE:CE2	2.56	0.40
1:B:462:THR:O	1:B:466:VAL:HG23	2.20	0.40
2:E:367:ASN:HB3	2:E:369:VAL:H	1.85	0.40
1:B:89:LEU:HD22	2:E:72:ASN:HA	2.04	0.40
1:B:71:MET:HE3	1:B:99:LYS:HB2	2.04	0.40
2:E:363:LEU:HD23	2:E:375:TRP:CE3	2.56	0.40
3:T:600:ILE:HG22	3:T:611:LYS:HG2	2.02	0.40
1:A:83:CYS:HB3	1:A:98:LEU:HG	2.02	0.40
2:E:319:PRO:HG2	2:E:326:ILE:HD12	2.04	0.40
2:E:118:ILE:HD11	2:E:422:ARG:HB2	2.03	0.40
1:B:457:LEU:HD23	3:S:678:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	450/643 (70%)	413 (92%)	33 (7%)	4 (1%)	21	64
1	B	452/643 (70%)	418 (92%)	32 (7%)	2 (0%)	39	80
2	E	356/362 (98%)	343 (96%)	11 (3%)	2 (1%)	30	72
2	F	357/362 (99%)	344 (96%)	11 (3%)	2 (1%)	30	72
3	S	126/191 (66%)	112 (89%)	13 (10%)	1 (1%)	24	66
3	T	126/191 (66%)	116 (92%)	9 (7%)	1 (1%)	24	66
All	All	1867/2392 (78%)	1746 (94%)	109 (6%)	12 (1%)	30	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	HIS
1	B	593	HIS
2	F	380	GLU
1	A	245	LYS
1	B	460	THR
2	E	380	GLU
3	S	579	MET
3	T	579	MET
1	A	273	GLN
1	A	565	GLN
2	E	174	GLY
2	F	174	GLY

5.3.2 Protein sidechains

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	419/560 (75%)	373 (89%)	46 (11%)	8	30
1	B	421/560 (75%)	377 (90%)	44 (10%)	8	32
2	E	321/325 (99%)	298 (93%)	23 (7%)	18	53
2	F	322/325 (99%)	297 (92%)	25 (8%)	16	49
3	S	122/175 (70%)	108 (88%)	14 (12%)	7	28
3	T	122/175 (70%)	109 (89%)	13 (11%)	8	31
All	All	1727/2120 (82%)	1562 (90%)	165 (10%)	10	38

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	LYS
1	A	25	ARG
1	A	28	GLN
1	A	29	LEU
1	A	34	ARG
1	A	36	ASP
1	A	51	GLU
1	A	53	THR
1	A	62	GLN
1	A	65	ILE
1	A	70	ILE
1	A	71	MET
1	A	86	THR
1	A	90	ASP
1	A	96	ILE
1	A	98	LEU
1	A	112	SER
1	A	116	LEU
1	A	117	GLN
1	A	198	GLU
1	A	225	GLU
1	A	239	GLU
1	A	241	LYS
1	A	243	LYS
1	A	275	GLU
1	A	287	ARG
1	A	444	ILE

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Mol	Chain	Res	Type
1	A	452	CYS
1	A	463	CYS
1	A	469	PHE
1	A	521	GLN
1	A	525	HIS
1	A	561	ARG
1	A	562	CYS
1	A	563	LYS
1	A	567	ASN
1	A	569	LYS
1	A	592	ASP
1	A	595	ASP
1	A	605	SER
1	A	611	LYS
1	A	628	ILE
1	A	632	VAL
1	A	675	VAL
1	A	685	ARG
1	B	13	ILE
1	B	14	CYS
1	B	27	ARG
1	B	28	GLN
1	B	29	LEU
1	B	33	ARG
1	B	39	LYS
1	B	51	GLU
1	B	53	THR
1	B	65	ILE
1	B	71	MET
1	B	86	THR
1	B	90	ASP
1	B	96	ILE
1	B	98	LEU
1	B	112	SER
1	B	116	LEU
1	B	117	GLN
1	B	198	GLU
1	B	239	GLU
1	B	241	LYS
1	B	245	LYS
1	B	274	ARG
1	B	275	GLU

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Mol	Chain	Res	Type
1	B	287	ARG
1	B	452	CYS
1	B	463	CYS
1	B	469	PHE
1	B	521	GLN
1	B	525	HIS
1	B	561	ARG
1	B	563	LYS
1	B	567	ASN
1	B	569	LYS
1	B	595	ASP
1	B	605	SER
1	B	611	LYS
1	B	628	ILE
1	B	632	VAL
1	B	670	ASN
1	B	672	ASP
1	B	675	VAL
1	B	685	ARG
1	B	732	ASP
2	E	101	THR
2	E	119	ARG
2	E	145	SER
2	E	177	ASN
2	E	182	LEU
2	E	201	LEU
2	E	246	LEU
2	E	254	LYS
2	E	255	ARG
2	E	261	LYS
2	E	325	ASP
2	E	326	ILE
2	E	329	ILE
2	E	330	LYS
2	E	341	ARG
2	E	348	ASP
2	E	356	MET
2	E	363	LEU
2	E	380	GLU
2	E	381	ASP
2	E	388	THR
2	E	408	SER

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Mol	Chain	Res	Type
2	E	415	CYS
2	F	101	THR
2	F	119	ARG
2	F	145	SER
2	F	177	ASN
2	F	182	LEU
2	F	201	LEU
2	F	246	LEU
2	F	254	LYS
2	F	255	ARG
2	F	261	LYS
2	F	326	ILE
2	F	328	LYS
2	F	329	ILE
2	F	330	LYS
2	F	341	ARG
2	F	348	ASP
2	F	356	MET
2	F	363	LEU
2	F	380	GLU
2	F	381	ASP
2	F	388	THR
2	F	390	LEU
2	F	408	SER
2	F	425	ARG
2	F	426	LEU
3	S	572	LEU
3	S	573	PRO
3	S	577	GLN
3	S	585	ASP
3	S	586	GLU
3	S	587	LYS
3	S	590	GLU
3	S	607	ASN
3	S	638	LEU
3	S	640	VAL
3	S	661	VAL
3	S	671	ILE
3	S	674	ILE
3	S	687	LYS
3	T	572	LEU
3	T	574	LEU

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Mol	Chain	Res	Type
3	T	585	ASP
3	T	586	GLU
3	T	587	LYS
3	T	590	GLU
3	T	607	ASN
3	T	638	LEU
3	T	640	VAL
3	T	661	VAL
3	T	671	ILE
3	T	674	ILE
3	T	687	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	263	ASN
1	A	607	GLN
1	A	648	GLN
1	A	670	ASN
1	B	57	ASN
1	B	94	GLN
1	B	263	ASN
1	B	565	GLN
1	B	567	ASN
1	B	607	GLN
1	B	648	GLN
1	B	668	ASN
1	B	670	ASN
1	B	706	HIS
2	E	175	HIS
2	E	291	HIS
2	E	360	GLN
2	E	367	ASN
2	F	175	HIS
2	F	291	HIS
2	F	360	GLN
2	F	367	ASN
3	S	562	ASN
3	S	607	ASN
3	S	631	GLN
3	S	642	ASN

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Mol	Chain	Res	Type
3	S	645	GLN
3	S	659	HIS
3	S	664	HIS
3	T	607	ASN
3	T	631	GLN
3	T	642	ASN
3	T	645	GLN
3	T	659	HIS

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 16 ligands modelled in this entry, 14 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	$\# Z > 2$
4	6BN	A	9001	-	36,39,39	0.94	2 (5%)	42,57,57	0.92	2 (4%)
4	6BN	B	9001	-	36,39,39	0.92	2 (5%)	42,57,57	0.92	2 (4%)

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
4	6BN	A	9001	-	-	0/18/41/41	0/4/4/4
4	6BN	B	9001	-	-	0/18/41/41	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	9001	6BN	C15-C14	2.77	1.44	1.39
4	A	9001	6BN	C15-C14	2.93	1.44	1.39
4	A	9001	6BN	C18-N17	3.43	1.39	1.33
4	B	9001	6BN	C18-N17	3.53	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	9001	6BN	C12-C13-C18	-2.57	114.95	119.07
4	B	9001	6BN	C12-C13-C18	-2.52	115.02	119.07
4	B	9001	6BN	C1-O25-C26	2.16	125.58	119.68
4	A	9001	6BN	C1-O25-C26	2.19	125.65	119.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	464/643 (72%)	0.34	22 (4%)	35 14	39, 66, 109, 139	0
1	B	466/643 (72%)	0.44	24 (5%)	31 12	41, 72, 113, 125	0
2	E	358/362 (98%)	0.26	4 (1%)	82 58	37, 59, 87, 127	0
2	F	359/362 (99%)	0.18	5 (1%)	78 51	35, 56, 87, 120	0
3	S	128/191 (67%)	0.41	4 (3%)	52 24	47, 83, 111, 117	0
3	T	128/191 (67%)	0.46	5 (3%)	43 18	41, 80, 112, 128	0
All	All	1903/2392 (79%)	0.33	64 (3%)	49 21	35, 65, 108, 139	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	THR	6.7
1	B	301	ALA	6.3
2	E	383	HIS	5.6
1	A	166	ILE	5.3
1	B	304	ASN	5.1
1	B	302	THR	4.1
1	B	300	HIS	3.9
1	B	166	ILE	3.7
1	B	446	THR	3.5
1	A	300	HIS	3.3
1	B	299	PHE	3.3
1	A	466	VAL	3.2
1	A	457	LEU	3.2
1	A	432	TRP	3.2
1	A	305	THR	3.2
1	B	307	LYS	3.1
1	B	303	PRO	3.0
1	B	281	PHE	2.9
1	B	306	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	466	VAL	2.9
3	S	640	VAL	2.8
2	F	381	ASP	2.8
1	B	439	MET	2.8
1	A	468	GLU	2.8
1	B	23	TYR	2.8
1	A	303	PRO	2.7
3	T	681	LEU	2.6
1	A	733	ALA	2.6
1	B	457	LEU	2.6
3	S	674	ILE	2.6
2	F	382	PRO	2.6
2	E	382	PRO	2.5
1	A	299	PHE	2.5
1	B	298	PRO	2.5
2	E	385	ALA	2.5
2	F	385	ALA	2.4
1	B	467	TYR	2.4
3	T	674	ILE	2.4
1	B	539	ALA	2.4
1	A	238	GLU	2.4
2	E	353	ARG	2.3
3	T	655	ASN	2.2
1	A	264	ILE	2.2
1	A	467	TYR	2.2
1	A	241	LYS	2.2
3	T	640	VAL	2.2
3	S	658	LEU	2.2
1	A	224	PHE	2.2
2	F	107	VAL	2.2
1	B	527	ARG	2.2
1	B	240	LEU	2.1
3	T	658	LEU	2.1
1	B	548	GLN	2.1
1	B	538	ILE	2.1
1	A	302	THR	2.1
2	F	383	HIS	2.1
3	S	579	MET	2.1
1	A	301	ALA	2.0
1	A	71	MET	2.0
1	A	527	ARG	2.0
1	A	275	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	2.0
1	A	442	VAL	2.0
1	A	304	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	ZN	A	9005	1/1	0.96	0.57	7.22	300,300,300,300	1
5	ZN	B	9007	1/1	0.98	0.21	2.28	65,65,65,65	1
5	ZN	A	9007	1/1	0.99	0.22	1.53	39,39,39,39	1
5	ZN	B	9006	1/1	0.99	0.21	1.07	53,53,53,53	1
5	ZN	A	9004	1/1	0.98	0.19	0.87	45,45,45,45	1
5	ZN	A	9006	1/1	0.99	0.20	0.83	37,37,37,37	1
5	ZN	A	9002	1/1	1.00	0.21	0.76	59,59,59,59	1
5	ZN	B	9008	1/1	0.99	0.21	0.48	47,47,47,47	1
5	ZN	B	9005	1/1	0.99	0.22	0.45	42,42,42,42	1
4	6BN	B	9001	36/36	0.96	0.24	0.42	29,50,68,69	0
5	ZN	A	9008	1/1	0.99	0.20	0.35	35,35,35,35	1
5	ZN	B	9004	1/1	0.95	0.21	0.31	59,59,59,59	1
4	6BN	A	9001	36/36	0.96	0.22	0.16	18,46,55,56	0
5	ZN	A	9003	1/1	1.00	0.18	0.10	45,45,45,45	1
5	ZN	B	9002	1/1	0.98	0.20	-0.08	53,53,53,53	1
5	ZN	B	9003	1/1	0.99	0.18	-0.40	61,61,61,61	1

6.5 Other polymers [i](#)

There are no such residues in this entry.