



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:31 am GMT

PDB ID : 5EUO  
Title : PF6-M1-HLA-A2  
Authors : Yang, X.  
Deposited on : 2015-11-18  
Resolution : 2.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

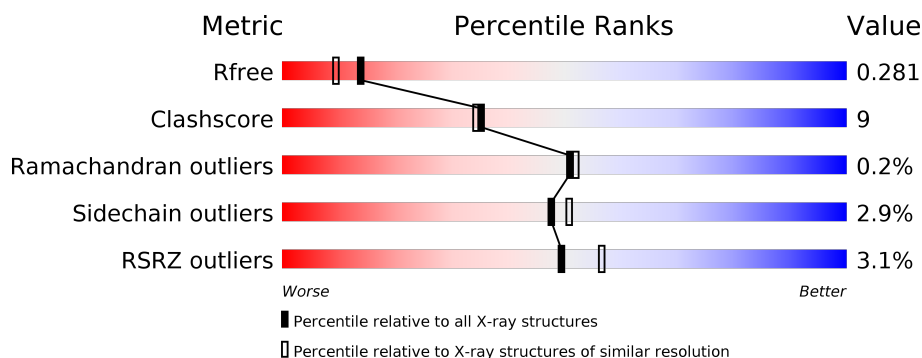
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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  $\geq 3$ , 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	276	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>...</div> </div> </div>
1	C	276	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	100	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
2	D	100	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
3	E	208	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>.</div> <div>9%</div> </div> </div>
3	G	208	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>.</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	240	<div><div>%</div><div><div></div><div>88%</div><div>11%</div></div></div>
4	H	240	<div><div>2%</div><div><div></div><div>71%</div><div>25%</div><div>• •</div></div></div>
5	I	9	<div><div></div><div><div>78%</div><div>22%</div></div></div>
5	J	9	<div><div></div><div><div>89%</div><div>11%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13444 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2237	1398	408	422	9			
1	C	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01892
C	0	MET	-	initiating methionine	UNP P01892

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
D	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called PF6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	190	Total	C	N	O	S	0	0	0
			1454	910	245	292	7			
3	G	191	Total	C	N	O	S	0	0	0
			1460	913	246	294	7			

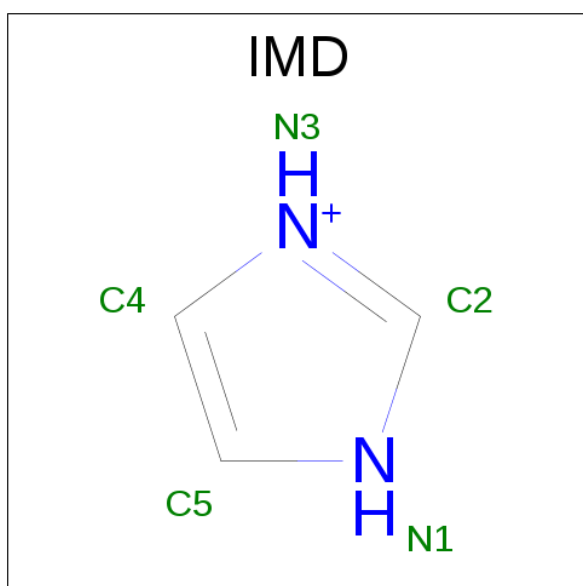
- Molecule 4 is a protein called PF6 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	239	Total	C	N	O	S	0	0	0
			1922	1214	332	370	6			
4	H	237	Total	C	N	O	S	0	0	0
			1906	1205	327	368	6			

- Molecule 5 is a protein called Matrix protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	0	0	0
			69	49	9	11			
5	J	9	Total	C	N	O	0	0	0
			69	49	9	11			

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			5	3	2		
6	G	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		

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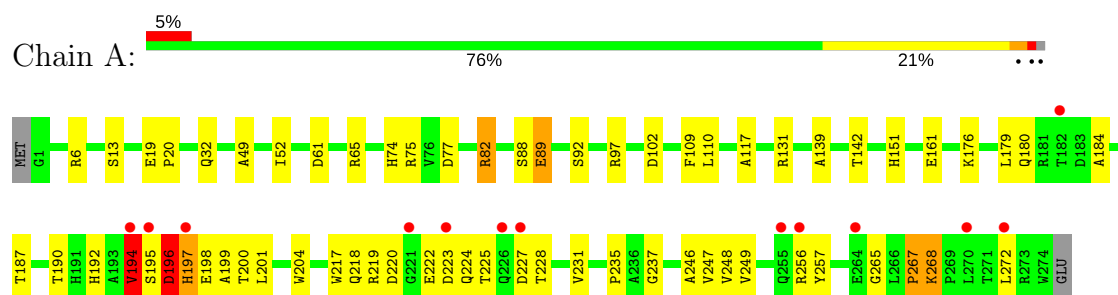
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total 11	O 11	0	0
7	C	96	Total 96	O 96	0	0
7	D	23	Total 23	O 23	0	0
7	E	29	Total 29	O 29	0	0
7	F	80	Total 80	O 80	0	0
7	G	38	Total 38	O 38	0	0
7	H	83	Total 83	O 83	0	0
7	I	6	Total 6	O 6	0	0
7	J	3	Total 3	O 3	0	0

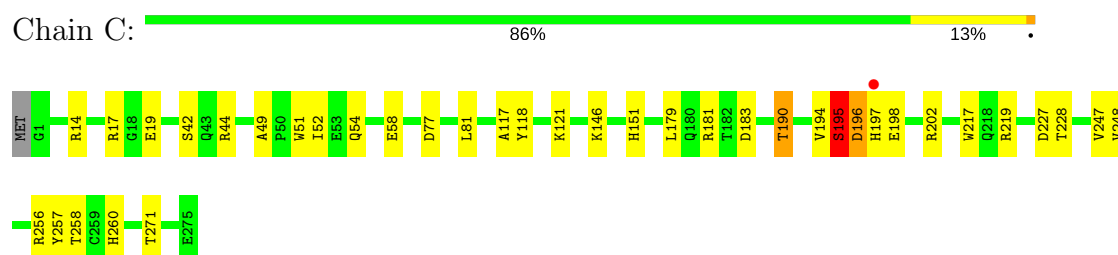
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

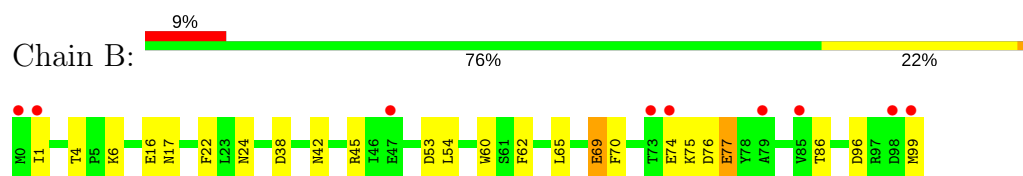
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



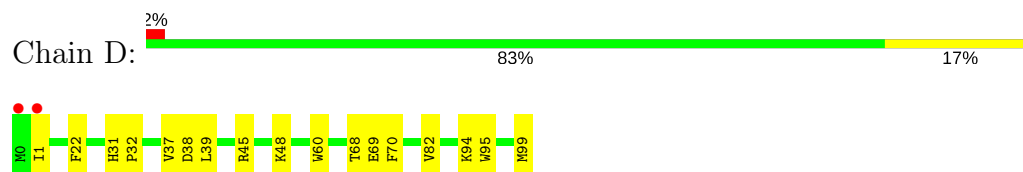
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin

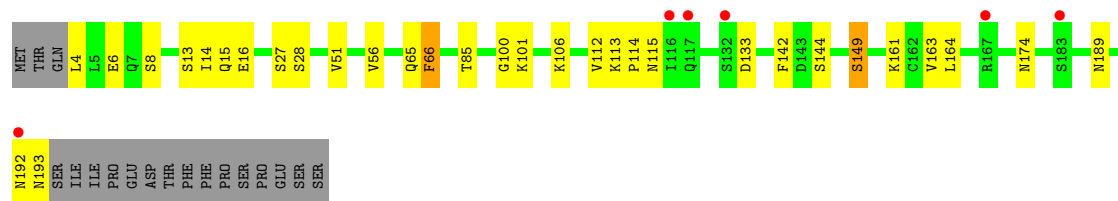


- Molecule 2: Beta-2-microglobulin

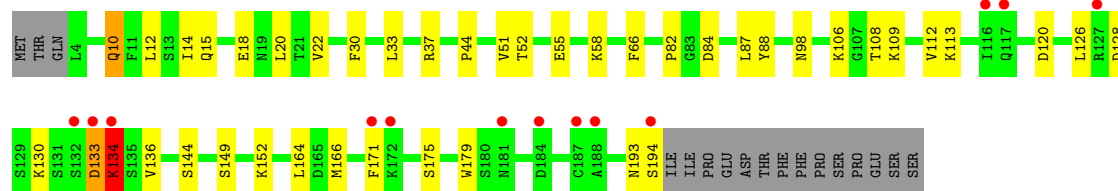


- Molecule 3: PF6 TCR alpha chain

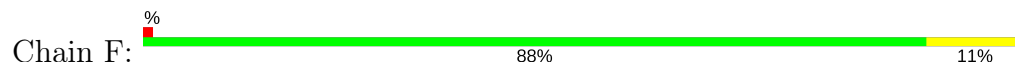




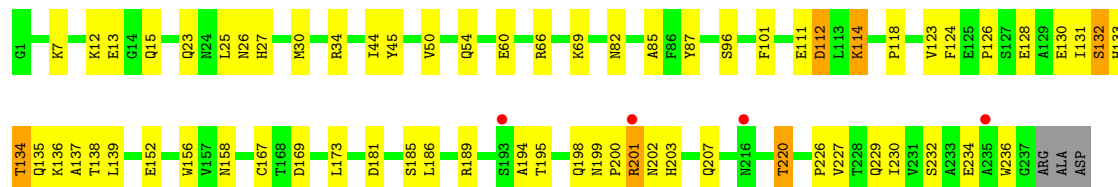
• Molecule 3: PF6 TCR alpha chain



• Molecule 4: PF6 TCR beta chain



• Molecule 4: PF6 TCR beta chain



• Molecule 5: Matrix protein 1



• Molecule 5: Matrix protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.74Å 54.08Å 149.30Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	120.47 – 2.10 120.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (120.47-2.10) 99.9 (120.47-2.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.229 , 0.281 0.230 , 0.281	Depositor DCC
$R_{free}$ test set	1978 reflections (1.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6143e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMD

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	0.49	0/2302	0.72	6/3125 (0.2%)
1	C	0.51	0/2312	0.60	0/3137
2	B	0.42	0/859	0.55	0/1162
2	D	0.52	0/860	0.61	0/1162
3	E	0.47	0/1481	0.65	1/2004 (0.0%)
3	G	0.57	0/1487	0.72	3/2012 (0.1%)
4	F	0.50	0/1975	0.61	0/2688
4	H	0.51	0/1959	0.61	1/2667 (0.0%)
5	I	0.51	0/70	0.68	0/92
5	J	0.58	0/70	0.65	0/92
All	All	0.50	0/13375	0.64	11/18141 (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	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	HIS	O-C-N	11.49	141.08	122.70
1	A	196	ASP	O-C-N	-9.21	107.96	122.70
1	A	194	VAL	O-C-N	-8.76	108.68	122.70
1	A	197	HIS	CA-C-N	-8.42	98.68	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	164	LEU	CA-CB-CG	6.42	130.05	115.30
1	A	194	VAL	CA-C-N	6.22	130.88	117.20
1	A	196	ASP	C-N-CA	-6.02	106.65	121.70
3	G	133	ASP	C-N-CA	5.58	135.65	121.70
4	H	173	LEU	CA-CB-CG	5.33	127.57	115.30
3	G	133	ASP	O-C-N	-5.33	114.17	122.70
3	G	134	LYS	CA-C-N	-5.01	106.18	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ASP	Mainchain
3	G	134	LYS	Mainchain

## 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	2237	0	2089	60	3
1	C	2247	0	2096	33	0
2	B	836	0	803	18	0
2	D	837	0	803	11	0
3	E	1454	0	1418	23	0
3	G	1460	0	1421	37	0
4	F	1922	0	1825	20	0
4	H	1906	0	1807	54	2
5	I	69	0	75	2	0
5	J	69	0	75	2	0
6	C	5	0	5	0	0
6	G	5	0	5	0	0
7	A	28	0	0	0	0
7	B	11	0	0	1	0
7	C	96	0	0	2	0
7	D	23	0	0	0	0
7	E	29	0	0	0	0
7	F	80	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	38	0	0	3	0
7	H	83	0	0	4	0
7	I	6	0	0	1	0
7	J	3	0	0	0	0
All	All	13444	0	12422	236	3

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 9.

All (236) 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:195:SER:O	1:A:197:HIS:N	1.79	1.14
1:A:219:ARG:HD3	1:A:256:ARG:HH12	1.03	1.10
1:A:194:VAL:HG12	1:A:195:SER:H	1.28	0.99
1:A:196:ASP:O	1:A:198:GLU:N	1.95	0.98
1:A:219:ARG:CD	1:A:256:ARG:HH12	1.76	0.96
4:H:30:MET:SD	7:H:379:HOH:O	2.22	0.96
1:A:219:ARG:HD3	1:A:256:ARG:NH1	1.80	0.95
3:E:85:THR:HG22	3:E:112:VAL:H	1.34	0.93
4:H:134:THR:HG23	4:H:136:LYS:H	1.31	0.92
1:A:222:GLU:CG	1:A:223:ASP:H	1.83	0.90
1:C:190:THR:HG22	1:C:202:ARG:HB3	1.55	0.89
3:G:128:ASP:OD2	7:G:401:HOH:O	1.91	0.89
4:F:110:THR:OG1	4:F:181:ASP:OD2	1.90	0.88
1:A:194:VAL:HG21	1:A:200:THR:OG1	1.77	0.85
3:G:164:LEU:HB3	4:H:167:CYS:HB2	1.60	0.83
4:H:23:GLN:HE21	4:H:25:LEU:H	1.25	0.82
1:A:220:ASP:OD1	1:A:256:ARG:HG2	1.80	0.81
1:C:195:SER:OG	1:C:196:ASP:N	2.13	0.81
1:C:228:THR:HG22	1:C:247:VAL:HG12	1.61	0.79
1:A:187:THR:HB	1:A:272:LEU:HD11	1.65	0.79
1:A:225:THR:O	1:A:228:THR:HG22	1.84	0.77
1:A:220:ASP:OD1	1:A:256:ARG:HD2	1.85	0.77
4:H:207:GLN:HE21	4:H:230:ILE:HD12	1.51	0.75
4:H:34:ARG:HB2	4:H:44:ILE:HD11	1.67	0.75
3:G:37:ARG:NH2	3:G:88:TYR:OH	2.20	0.74
2:D:39:LEU:HD12	2:D:68:THR:HG22	1.68	0.73
4:H:23:GLN:HE21	4:H:25:LEU:N	1.86	0.73
3:E:142:PHE:HE2	3:E:161:LYS:HE3	1.55	0.72
1:A:194:VAL:CG2	1:A:200:THR:OG1	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	1:A:224:GLN:N	2.24	0.70
3:E:13:SER:OG	3:E:113:LYS:HE2	1.92	0.70
1:A:190:THR:HG22	1:A:192:HIS:CE1	2.26	0.69
1:A:222:GLU:HG2	1:A:223:ASP:H	1.56	0.69
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.73	0.69
2:B:42:ASN:ND2	2:B:76:ASP:OD1	2.21	0.69
4:H:34:ARG:NH2	4:H:82:ASN:O	2.26	0.68
3:G:10:GLN:H	3:G:10:GLN:CD	1.97	0.67
1:A:220:ASP:OD1	1:A:256:ARG:CG	2.43	0.66
1:A:222:GLU:HG3	1:A:223:ASP:H	1.57	0.66
1:A:222:GLU:CG	1:A:223:ASP:N	2.56	0.66
1:C:77:ASP:HB3	5:I:9:LEU:HD12	1.77	0.65
1:C:260:HIS:CD2	1:C:271:THR:HG22	2.32	0.64
2:B:42:ASN:HA	2:B:77:GLU:HG2	1.80	0.64
3:G:51:VAL:HG23	3:G:52:THR:HG23	1.80	0.64
1:A:220:ASP:OD1	1:A:256:ARG:CD	2.45	0.63
7:C:405:HOH:O	3:G:52:THR:HG22	1.97	0.63
3:E:189:ASN:O	3:E:192:ASN:ND2	2.31	0.63
4:H:123:VAL:HG13	4:H:139:LEU:HD21	1.79	0.62
2:B:17:ASN:HD21	2:B:74:GLU:N	1.97	0.62
4:H:50:VAL:HG23	7:H:341:HOH:O	1.99	0.62
1:A:190:THR:CG2	1:A:192:HIS:HE1	2.12	0.62
1:A:194:VAL:HG12	1:A:195:SER:N	1.97	0.62
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.33	0.62
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.83	0.61
1:C:194:VAL:O	1:C:194:VAL:HG12	2.00	0.61
4:H:23:GLN:NE2	4:H:27:HIS:H	1.98	0.61
2:B:17:ASN:HD21	2:B:74:GLU:H	1.48	0.60
1:A:219:ARG:CG	1:A:256:ARG:HH12	2.13	0.60
1:A:190:THR:HG22	1:A:192:HIS:HE1	1.65	0.60
4:H:12:LYS:HB3	4:H:15:GLN:HE21	1.66	0.60
4:F:203:HIS:HB2	4:F:236:TRP:CZ3	2.38	0.59
3:G:37:ARG:HH12	3:G:84:ASP:HA	1.67	0.59
3:G:166:MET:SD	3:G:171:PHE:HD2	2.26	0.58
1:C:14:ARG:NE	1:C:19:GLU:O	2.26	0.58
1:A:195:SER:O	1:A:196:ASP:C	2.41	0.58
2:B:4:THR:HA	2:B:86:THR:HG21	1.85	0.58
1:A:77:ASP:HB3	5:J:9:LEU:HD12	1.86	0.58
2:B:22:PHE:CZ	2:B:69:GLU:HG3	2.39	0.57
3:G:87:LEU:HD12	3:G:109:LYS:HG3	1.87	0.57
4:F:176:GLN:HE21	4:F:178:ALA:H	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:THR:HG22	7:C:423:HOH:O	2.04	0.57
1:C:181:ARG:NH1	1:C:183:ASP:OD2	2.38	0.56
3:G:37:ARG:NH2	3:G:88:TYR:CZ	2.73	0.56
2:D:22:PHE:CE1	2:D:69:GLU:HB3	2.39	0.56
3:E:13:SER:OG	3:E:113:LYS:CE	2.53	0.56
4:H:23:GLN:NE2	4:H:25:LEU:H	1.99	0.56
4:F:10:PHE:O	4:F:11:ARG:NH1	2.37	0.56
3:G:120:ASP:OD2	4:H:133:HIS:HE1	1.88	0.56
1:C:195:SER:OG	1:C:197:HIS:N	2.38	0.56
3:G:37:ARG:NH1	3:G:84:ASP:HA	2.20	0.56
2:B:22:PHE:CE2	2:B:69:GLU:HG3	2.41	0.56
4:F:176:GLN:NE2	4:F:178:ALA:HB3	2.20	0.56
1:A:82:ARG:HH12	1:A:89:GLU:HB3	1.70	0.56
1:C:258:THR:HG23	1:C:260:HIS:HE1	1.71	0.55
4:H:130:GLU:O	4:H:134:THR:HG22	2.06	0.55
4:H:194:ALA:O	4:H:198:GLN:HG2	2.06	0.55
3:E:15:GLN:NE2	3:E:113:LYS:HB2	2.22	0.55
1:A:227:ASP:HB3	1:A:248:VAL:HG22	1.88	0.54
2:B:38:ASP:OD1	2:B:45:ARG:NH1	2.36	0.54
4:F:176:GLN:O	4:F:176:GLN:HG3	2.06	0.54
4:H:195:THR:O	4:H:199:ASN:ND2	2.40	0.54
4:H:7:LYS:NZ	4:H:152:GLU:OE2	2.33	0.54
1:C:227:ASP:HB3	1:C:248:VAL:HG22	1.90	0.54
3:E:56:VAL:HG22	3:E:65:GLN:HG3	1.89	0.54
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.89	0.54
4:H:207:GLN:NE2	4:H:230:ILE:HD12	2.22	0.53
1:C:258:THR:HG23	1:C:260:HIS:CE1	2.44	0.53
3:G:98:ASN:O	5:I:4:GLY:HA3	2.09	0.53
4:H:128:GLU:O	4:H:132:SER:HB3	2.09	0.52
3:E:14:ILE:O	3:E:112:VAL:HA	2.10	0.52
1:A:19:GLU:HG2	1:A:75:ARG:HH21	1.75	0.51
4:H:30:MET:HE2	4:H:69:LYS:O	2.10	0.51
1:C:14:ARG:HH11	1:C:17:ARG:HH12	1.57	0.51
3:G:52:THR:OG1	3:G:55:GLU:HB2	2.10	0.51
4:H:13:GLU:HG2	4:H:111:GLU:HA	1.92	0.51
3:E:16:GLU:OE2	3:E:115:ASN:HB2	2.11	0.51
1:A:32:GLN:NE2	2:B:53:ASP:OD2	2.39	0.51
1:C:117:ALA:HB2	2:D:60:TRP:CE2	2.45	0.51
4:H:195:THR:HG22	7:H:370:HOH:O	2.11	0.51
3:G:106:LYS:NZ	7:G:402:HOH:O	2.43	0.50
4:H:158:ASN:HD21	4:H:202:ASN:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:200:PRO:HA	4:H:202:ASN:N	2.26	0.50
3:G:179:TRP:HZ2	4:H:185:SER:HG	1.60	0.50
2:D:38:ASP:OD1	2:D:45:ARG:NH1	2.44	0.50
4:H:227:VAL:O	4:H:229:GLN:HG2	2.11	0.50
4:H:26:ASN:OD1	4:H:69:LYS:NZ	2.37	0.50
1:C:190:THR:HG21	2:D:99:MET:OXT	2.11	0.50
3:E:149:SER:OG	3:E:193:ASN:O	2.19	0.50
3:E:100:GLY:HA2	4:F:96:SER:HB2	1.93	0.50
4:H:23:GLN:HE22	4:H:27:HIS:H	1.59	0.50
1:C:58:GLU:H	1:C:58:GLU:CD	2.14	0.49
4:H:131:ILE:HG23	4:H:194:ALA:HB1	1.94	0.49
3:G:152:LYS:H	3:G:193:ASN:HD22	1.61	0.49
3:E:101:LYS:HE3	7:F:305:HOH:O	2.11	0.49
1:C:202:ARG:HD2	2:D:99:MET:OXT	2.12	0.49
1:A:219:ARG:HG3	1:A:257:TYR:HE1	1.78	0.49
1:C:151:HIS:CE1	3:G:51:VAL:HG21	2.48	0.49
1:C:217:TRP:CD1	1:C:247:VAL:HG13	2.48	0.49
4:H:135:GLN:OE1	4:H:136:LYS:NZ	2.43	0.49
3:G:152:LYS:H	3:G:193:ASN:ND2	2.10	0.49
1:A:151:HIS:ND1	3:E:51:VAL:HG11	2.28	0.49
2:B:96:ASP:OD2	2:B:99:MET:HE2	2.13	0.49
3:G:82:PRO:HA	3:G:112:VAL:HB	1.95	0.49
1:A:190:THR:CG2	1:A:192:HIS:CE1	2.91	0.48
1:C:219:ARG:HG3	1:C:257:TYR:CZ	2.49	0.48
4:H:156:TRP:NE1	4:H:207:GLN:OE1	2.46	0.48
1:C:121:LYS:HG3	2:D:1:ILE:HG12	1.96	0.48
4:F:111:GLU:O	4:F:112:ASP:HB2	2.12	0.48
2:D:48:LYS:HB3	2:D:48:LYS:HE3	1.72	0.47
4:F:112:ASP:OD2	4:F:114:LYS:HG2	2.14	0.47
4:F:147:TYR:CZ	4:F:181:ASP:HB3	2.50	0.47
3:G:15:GLN:O	3:G:18:GLU:HG2	2.14	0.47
2:D:37:VAL:HG22	2:D:82:VAL:HG22	1.96	0.47
4:F:112:ASP:CG	4:F:114:LYS:HG2	2.35	0.47
1:A:267:PRO:HB2	1:A:268:LYS:HG3	1.96	0.47
3:E:106:LYS:NZ	4:F:40:GLY:HA3	2.29	0.47
4:H:112:ASP:OD2	4:H:114:LYS:HB3	2.15	0.47
3:E:16:GLU:OE2	3:E:115:ASN:N	2.35	0.47
4:H:60:GLU:H	4:H:60:GLU:CD	2.17	0.47
4:H:135:GLN:CD	4:H:135:GLN:H	2.18	0.47
4:H:30:MET:HE3	4:H:66:ARG:NE	2.30	0.46
4:F:147:TYR:CD1	4:F:148:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:30:MET:HE2	4:F:69:LYS:O	2.16	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.46
1:C:219:ARG:HH11	1:C:256:ARG:NH2	2.13	0.46
3:E:163:VAL:HG22	3:E:174:ASN:OD1	2.15	0.46
3:E:15:GLN:HG2	3:E:113:LYS:HB2	1.98	0.46
1:C:81:LEU:HD13	1:C:118:TYR:CD1	2.50	0.46
4:F:195:THR:HG23	7:F:358:HOH:O	2.15	0.46
1:A:237:GLY:HA3	7:B:101:HOH:O	2.14	0.46
2:B:75:LYS:HG3	2:B:75:LYS:O	2.16	0.46
3:E:85:THR:HG22	3:E:112:VAL:N	2.16	0.46
1:A:74:HIS:NE2	1:A:97:ARG:HD2	2.31	0.45
1:C:51:TRP:O	1:C:54:GLN:HG2	2.15	0.45
4:H:50:VAL:HG22	4:H:69:LYS:HA	1.99	0.45
1:C:17:ARG:HG2	1:C:17:ARG:O	2.16	0.45
3:G:58:LYS:HE3	3:G:58:LYS:HB3	1.78	0.45
4:H:200:PRO:CB	4:H:201:ARG:HA	2.47	0.45
4:H:169:ASP:HB2	4:H:186:LEU:HD12	1.98	0.45
1:A:194:VAL:O	1:A:196:ASP:N	2.49	0.45
2:B:69:GLU:O	2:B:70:PHE:HD1	2.00	0.45
1:C:14:ARG:HD2	1:C:17:ARG:NH1	2.32	0.45
4:H:130:GLU:CD	4:H:138:THR:H	2.19	0.44
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.82	0.44
4:F:182:SER:N	7:F:303:HOH:O	2.46	0.44
1:A:204:TRP:HH2	2:B:99:MET:O	2.00	0.44
1:C:49:ALA:O	1:C:52:ILE:HG22	2.17	0.44
4:F:112:ASP:OD2	4:F:114:LYS:HD2	2.18	0.44
3:G:126:LEU:HG	4:H:126:PRO:HA	2.00	0.44
2:D:94:LYS:HG3	2:D:95:TRP:N	2.31	0.44
4:H:126:PRO:HG3	4:H:137:ALA:HB1	1.99	0.44
1:A:201:LEU:O	1:A:246:ALA:HA	2.18	0.44
1:A:139:ALA:O	1:A:142:THR:HB	2.18	0.43
2:B:6:LYS:HB2	2:B:6:LYS:HE3	1.83	0.43
4:H:23:GLN:NE2	7:H:311:HOH:O	2.50	0.43
3:G:106:LYS:HD3	3:G:106:LYS:HA	1.69	0.43
3:G:175:SER:OG	4:H:189:ARG:HD3	2.17	0.43
1:A:61:ASP:HB3	1:A:65:ARG:NH1	2.34	0.43
1:A:199:ALA:HB3	1:A:249:VAL:HG22	2.00	0.43
1:A:77:ASP:CG	5:J:9:LEU:HG	2.39	0.43
3:E:114:PRO:O	3:E:144:SER:OG	2.37	0.43
1:A:19:GLU:CG	1:A:20:PRO:HD2	2.46	0.43
1:A:200:THR:HA	1:A:247:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:113:LYS:HB3	3:E:144:SER:HB3	2.01	0.43
3:G:128:ASP:O	3:G:130:LYS:N	2.51	0.43
1:A:109:PHE:CZ	1:A:161:GLU:HG2	2.54	0.42
1:A:176:LYS:HG3	1:A:180:GLN:OE1	2.19	0.42
3:G:30:PHE:CE2	3:G:33:LEU:HD12	2.54	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.18	0.42
2:B:54:LEU:HD11	2:B:62:PHE:CD1	2.54	0.42
4:H:220:THR:O	4:H:220:THR:OG1	2.35	0.42
1:C:42:SER:O	1:C:44:ARG:HG2	2.18	0.42
3:G:10:GLN:O	3:G:109:LYS:HD2	2.20	0.42
1:A:184:ALA:HB2	1:A:265:GLY:O	2.19	0.42
1:A:217:TRP:O	1:A:218:GLN:HB2	2.18	0.42
1:C:51:TRP:CZ2	1:C:179:LEU:HD11	2.55	0.42
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.35	0.42
3:G:14:ILE:HD11	3:G:112:VAL:HG22	2.02	0.42
4:H:118:PRO:HD3	4:H:226:PRO:HB3	2.02	0.42
1:A:13:SER:O	1:A:92:SER:OG	2.23	0.42
1:C:258:THR:CG2	1:C:260:HIS:HE1	2.33	0.42
3:G:22:VAL:HG11	3:G:108:THR:HG21	2.01	0.42
4:H:85:ALA:HB3	4:H:87:TYR:CE1	2.55	0.42
3:G:120:ASP:OD2	4:H:133:HIS:CE1	2.71	0.42
1:A:219:ARG:HG2	1:A:256:ARG:NH1	2.35	0.41
1:C:190:THR:CG2	1:C:202:ARG:HB3	2.37	0.41
3:E:4:LEU:HD22	3:E:27:SER:HB3	2.02	0.41
3:G:44:PRO:HD2	4:H:101:PHE:CG	2.55	0.41
3:E:133:ASP:N	3:E:133:ASP:OD1	2.47	0.41
3:G:136:VAL:HG13	4:H:124:PHE:CE2	2.56	0.41
3:G:149:SER:HB3	3:G:194:SER:HB2	2.01	0.41
4:H:203:HIS:NE2	4:H:234:GLU:OE1	2.50	0.41
1:A:219:ARG:HG2	1:A:256:ARG:HH12	1.82	0.41
3:G:15:GLN:N	7:G:405:HOH:O	2.51	0.41
1:A:19:GLU:HG2	1:A:75:ARG:NH2	2.35	0.41
1:C:146:LYS:HE2	7:I:106:HOH:O	2.20	0.41
3:E:66:PHE:HA	3:E:66:PHE:HD1	1.75	0.40
4:H:30:MET:CE	4:H:66:ARG:NE	2.84	0.40
1:A:222:GLU:HG3	1:A:223:ASP:N	2.27	0.40
4:F:86:PHE:HD1	4:F:106:ARG:HG2	1.86	0.40
3:G:113:LYS:HB3	3:G:144:SER:HB3	2.02	0.40
4:H:199:ASN:O	4:H:202:ASN:HB2	2.21	0.40
4:H:236:TRP:N	4:H:236:TRP:CD1	2.90	0.40
4:F:2:ILE:HG23	4:F:23:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:133:ASP:O	3:G:134:LYS:HB2	2.21	0.40
4:F:219:TRP:CB	4:F:225:LYS:HE2	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:OD2	4:H:201:ARG:CB[2_16412]	1.62	0.58
1:A:131:ARG:NH2	1:A:198:GLU:OE2[2_15511]	1.62	0.58
1:A:220:ASP:OD2	4:H:201:ARG:CA[2_16412]	1.89	0.31

## 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	272/276 (99%)	251 (92%)	18 (7%)	3 (1%)	17	11
1	C	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	38	35
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	D	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	E	188/208 (90%)	179 (95%)	9 (5%)	0	100	100
3	G	189/208 (91%)	174 (92%)	15 (8%)	0	100	100
4	F	237/240 (99%)	230 (97%)	7 (3%)	0	100	100
4	H	235/240 (98%)	229 (97%)	6 (3%)	0	100	100
5	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
5	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1604/1666 (96%)	1530 (95%)	70 (4%)	4 (0%)	51	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	C	195	SER
1	A	194	VAL
1	A	267	PRO

### 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	230/232 (99%)	223 (97%)	7 (3%)	46	49
1	C	231/232 (100%)	227 (98%)	4 (2%)	66	72
2	B	95/95 (100%)	91 (96%)	4 (4%)	34	33
2	D	95/95 (100%)	94 (99%)	1 (1%)	78	83
3	E	166/184 (90%)	161 (97%)	5 (3%)	46	49
3	G	167/184 (91%)	162 (97%)	5 (3%)	46	49
4	F	210/211 (100%)	206 (98%)	4 (2%)	62	68
4	H	209/211 (99%)	198 (95%)	11 (5%)	26	24
5	I	7/7 (100%)	7 (100%)	0	100	100
5	J	7/7 (100%)	7 (100%)	0	100	100
All	All	1417/1458 (97%)	1376 (97%)	41 (3%)	48	51

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	88	SER
1	A	89	GLU
1	A	110	LEU
1	A	179	LEU
1	A	231	VAL
1	A	268	LYS
2	B	1	ILE
2	B	16	GLU
2	B	69	GLU

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Mol	Chain	Res	Type
2	B	77	GLU
1	C	190	THR
1	C	195	SER
1	C	196	ASP
1	C	198	GLU
2	D	70	PHE
3	E	6	GLU
3	E	8	SER
3	E	28	SER
3	E	66	PHE
3	E	149	SER
4	F	2	ILE
4	F	3	THR
4	F	60	GLU
4	F	189	ARG
3	G	10	GLN
3	G	12	LEU
3	G	20	LEU
3	G	66	PHE
3	G	134	LYS
4	H	45	TYR
4	H	54	GLN
4	H	96	SER
4	H	112	ASP
4	H	114	LYS
4	H	132	SER
4	H	134	THR
4	H	181	ASP
4	H	201	ARG
4	H	220	THR
4	H	232	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	255	GLN
1	A	260	HIS
2	B	17	ASN
1	C	260	HIS
4	F	176	GLN
3	G	34	GLN

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Mol	Chain	Res	Type
3	G	118	ASN
3	G	145	GLN
3	G	189	ASN
3	G	193	ASN
4	H	15	GLN
4	H	23	GLN
4	H	133	HIS
4	H	158	ASN
4	H	199	ASN
4	H	207	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
6	IMD	C	301	-	3,5,5	0.56	0	4,5,5	0.72	0
6	IMD	G	301	-	3,5,5	0.52	0	4,5,5	0.45	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
6	IMD	C	301	-	-	0/0/0/0	0/1/1/1
6	IMD	G	301	-	-	0/0/0/0	0/1/1/1

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.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/276 (99%)	0.32	13 (4%) 32 38	31, 50, 76, 86	0
1	C	275/276 (99%)	-0.13	1 (0%) 92 93	22, 36, 58, 76	0
2	B	100/100 (100%)	0.64	9 (9%) 10 13	40, 63, 76, 82	0
2	D	100/100 (100%)	0.01	2 (2%) 65 70	24, 45, 66, 74	0
3	E	190/208 (91%)	0.25	6 (3%) 48 55	31, 51, 72, 81	0
3	G	191/208 (91%)	0.42	13 (6%) 18 23	26, 51, 78, 88	0
4	F	239/240 (99%)	-0.15	2 (0%) 86 88	26, 38, 61, 70	0
4	H	237/240 (98%)	0.13	4 (1%) 70 75	21, 39, 68, 83	0
5	I	9/9 (100%)	-0.27	0 100 100	24, 26, 28, 32	0
5	J	9/9 (100%)	-0.23	0 100 100	31, 33, 36, 42	0
All	All	1624/1666 (97%)	0.14	50 (3%) 49 56	21, 44, 72, 88	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	0	MET	7.1
3	E	132	SER	5.9
4	H	201	ARG	5.6
1	A	221	GLY	5.5
3	G	184	ASP	5.2
1	A	197	HIS	4.9
1	A	195	SER	4.8
2	B	0	MET	4.6
2	B	99	MET	3.8
3	G	134	LYS	3.8
3	G	132	SER	3.7
2	B	79	ALA	3.7
1	A	227	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	E	117	GLN	3.3
1	A	270	LEU	3.3
3	E	183	SER	3.1
3	G	188	ALA	3.1
3	E	116	ILE	3.0
1	A	182	THR	3.0
1	A	272	LEU	2.9
2	D	1	ILE	2.8
1	C	197	HIS	2.8
4	F	215	GLU	2.8
1	A	223	ASP	2.7
2	B	47	GLU	2.6
3	G	133	ASP	2.6
3	E	192	ASN	2.5
2	B	85	VAL	2.5
3	G	194	SER	2.5
3	G	171	PHE	2.5
3	G	117	GLN	2.5
3	E	167	ARG	2.4
4	F	176	GLN	2.3
1	A	256	ARG	2.3
1	A	255	GLN	2.3
3	G	116	ILE	2.3
2	B	98	ASP	2.3
2	B	73	THR	2.3
4	H	216	ASN	2.3
1	A	194	VAL	2.2
4	H	235	ALA	2.2
2	B	1	ILE	2.2
3	G	172	LYS	2.1
4	H	193	SER	2.1
3	G	187	CYS	2.1
2	B	74	GLU	2.1
3	G	181	ASN	2.1
1	A	226	GLN	2.1
1	A	264	GLU	2.0
3	G	127	ARG	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 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	IMD	G	301	5/5	0.95	0.14	1.44	37,39,40,43	0
6	IMD	C	301	5/5	0.77	0.15	-	42,42,48,52	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.