



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:45 am BST

PDB ID : 3FFC  
Title : Crystal Structure of CF34 TCR in complex with HLA-B8/FLR  
Authors : Gras, S.; Burrows, S.R.; Kjer-Nielsen, L.; Clements, C.S.; Liu, Y.C.; Sullivan, L.C.; Brooks, A.G.; Purcell, A.W.; McCluskey, J.; Rossjohn, J.  
Deposited on : 2008-12-03  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

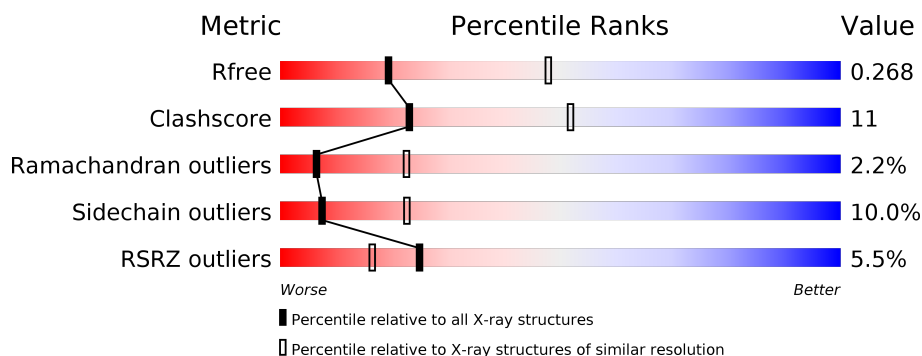
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	277	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>.</div> </div> </div>
1	F	277	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>5%</div> </div> </div>
2	B	100	<div> <div></div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
2	G	100	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>25%</div> <div>.</div> </div> </div>
3	C	9	<div> <div></div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
3	H	9	<div> <div></div> <div> <div></div> <div>78%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	202	
4	I	202	
5	E	247	
5	J	247	

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
7	CL	J	266	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13519 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, B-8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	2	0
			2278	1409	417	445	7			
1	F	276	Total	C	N	O	S	0	0	0
			2251	1395	411	438	7			

- 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	1	0
			848	539	145	160	4			
2	G	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
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called FLRGRAYGL peptide from an EBV protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	49	15	11			
3	H	9	Total	C	N	O	0	0	0
			75	49	15	11			

- Molecule 4 is a protein called CF34 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	202	Total	C	N	O	S	0	0	0
			1582	990	255	326	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	202	Total	C	N	O	S	0	2	0
			1602	1001	260	330	11			

- Molecule 5 is a protein called CF34 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	247	Total	C	N	O	S	0	0	0
			1964	1246	340	372	6			
5	J	247	Total	C	N	O	S	0	1	0
			1973	1251	341	375	6			

- Molecule 6 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Cd	0	0
			2	2		
6	J	1	Total	Cd	0	0
			1	1		
6	E	2	Total	Cd	0	0
			2	2		
6	B	2	Total	Cd	0	0
			2	2		
6	I	1	Total	Cd	0	0
			1	1		
6	A	1	Total	Cd	0	0
			1	1		
6	F	1	Total	Cd	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	0	0
			1	1		
7	J	3	Total	Cl	0	0
			3	3		
7	D	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	Cl 3	0	0
7	F	1	Total 1	Cl 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	2	Total 2	Na 2	0	0
8	J	2	Total 2	Na 2	0	0
8	D	1	Total 1	Na 1	0	0
8	E	1	Total 1	Na 1	0	0
8	B	2	Total 2	Na 2	0	0
8	A	2	Total 2	Na 2	0	0

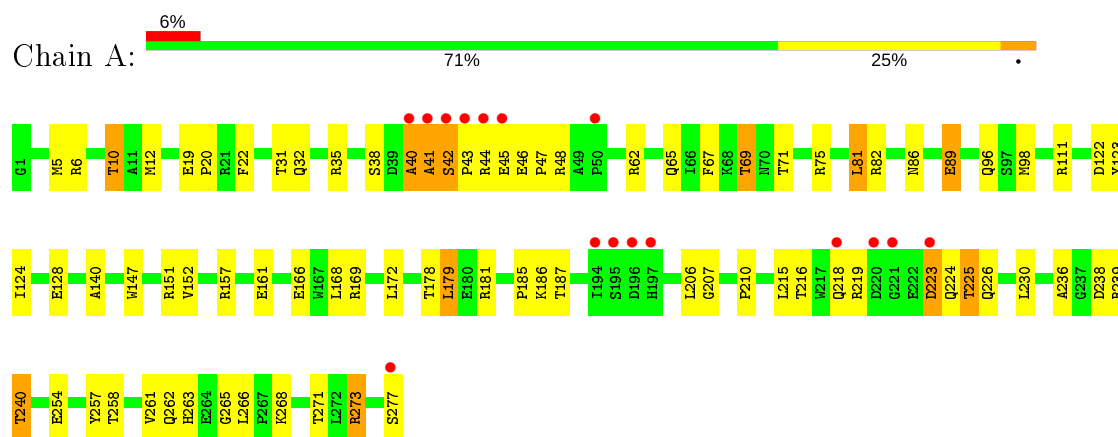
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	O 1	0	0
9	J	2	Total 2	O 2	0	0

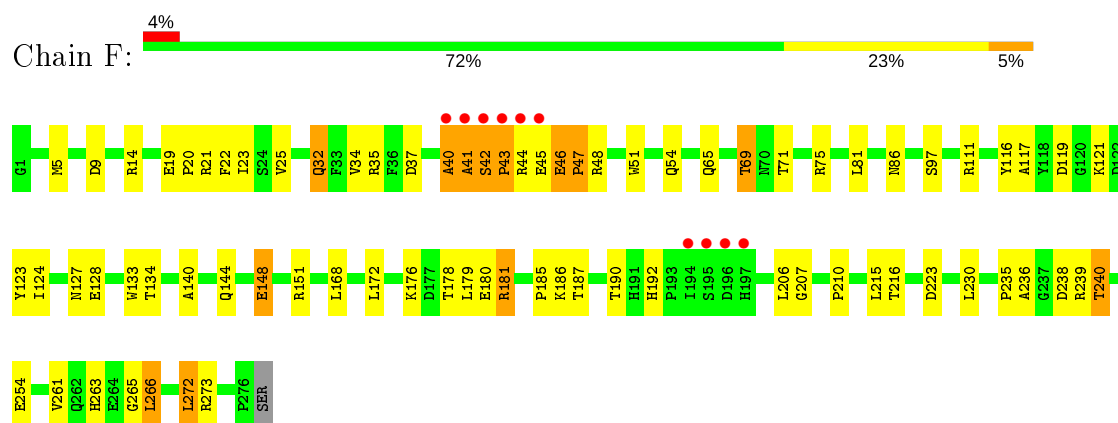
### 3 Residue-property plots [i](#)

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.

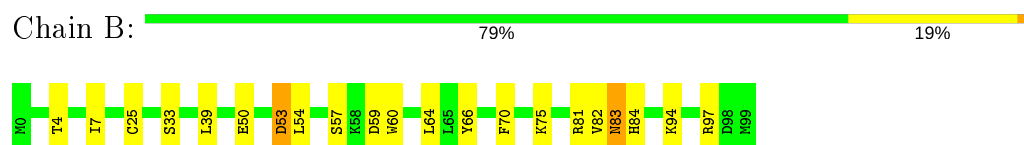
- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain



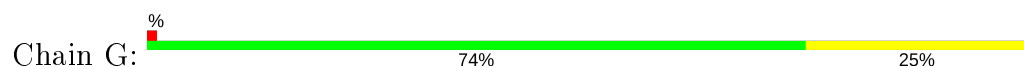
- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain



- Molecule 2: Beta-2-microglobulin

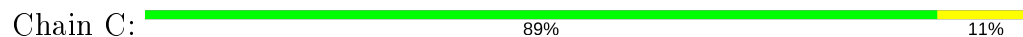


- Molecule 2: Beta-2-microglobulin

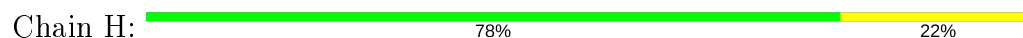




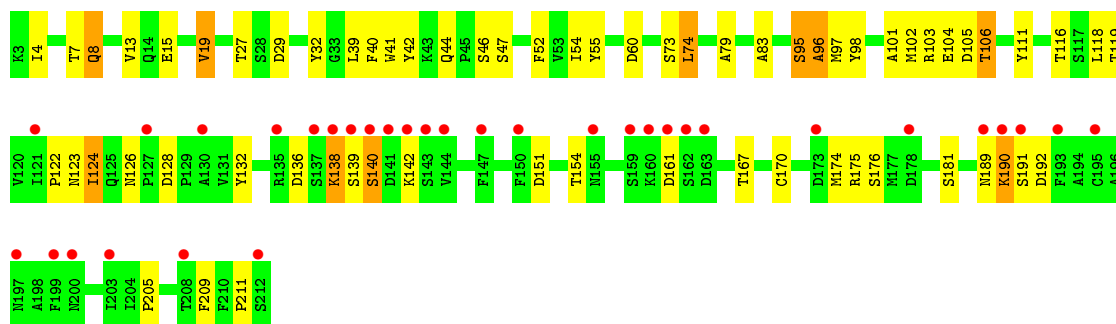
- Molecule 3: FLRGRAYGL peptide from an EBV protein



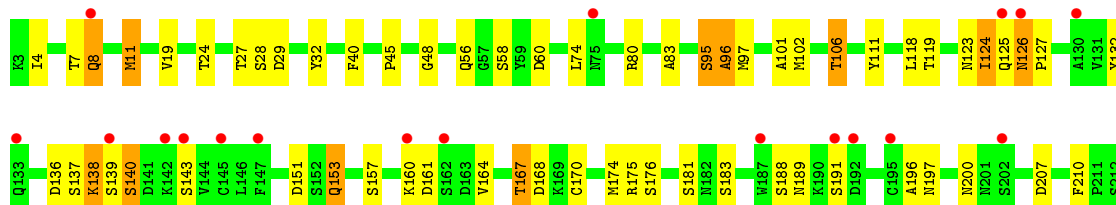
- Molecule 3: FLRGRAYGL peptide from an EBV protein



- Molecule 4: CF34 alpha chain



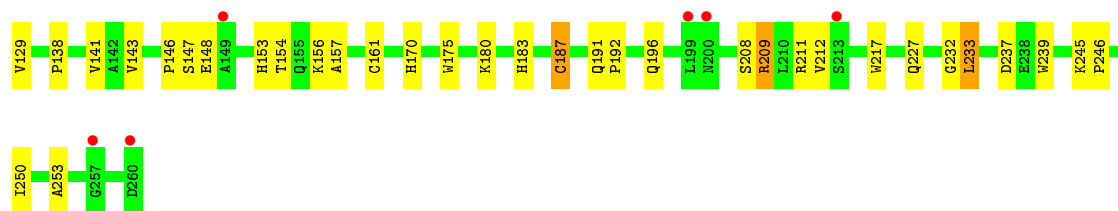
- Molecule 4: CF34 alpha chain



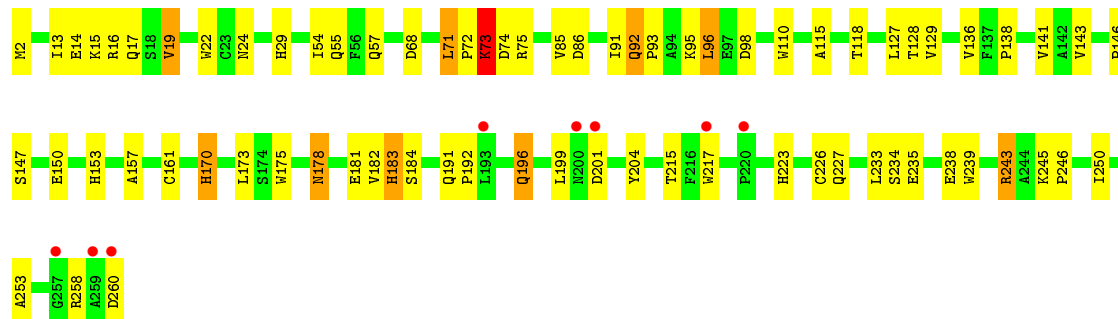
- Molecule 5: CF34 beta chain







● Molecule 5: CF34 beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.56Å 171.81Å 272.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 48.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.80) 99.9 (48.45-2.70)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.34	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.69Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.221 , 0.268 0.224 , 0.268	Depositor DCC
$R_{free}$ test set	3638 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.633	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.99 % 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 6.2519e-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: NA, CL, CD

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	0/2340	0.61	0/3180
1	F	0.46	0/2313	0.63	0/3146
2	B	0.51	0/871	0.64	0/1176
2	G	0.49	0/860	0.64	0/1162
3	C	0.46	0/76	0.62	0/98
3	H	0.49	0/76	0.68	0/98
4	D	0.43	0/1617	0.61	0/2189
4	I	0.44	0/1637	0.60	0/2215
5	E	0.47	0/2018	0.62	0/2748
5	J	0.48	0/2027	0.61	0/2760
All	All	0.46	0/13835	0.62	0/18772

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
5	E	0	1
5	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	92	GLN	Peptide

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Mol	Chain	Res	Type	Group
5	J	92	GLN	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	2278	0	2115	59	0
1	F	2251	0	2093	64	0
2	B	848	0	815	12	0
2	G	837	0	803	15	0
3	C	75	0	79	2	0
3	H	75	0	79	2	0
4	D	1582	0	1477	39	0
4	I	1602	0	1494	29	0
5	E	1964	0	1889	49	0
5	J	1973	0	1894	62	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	1	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	J	3	0	0	3	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	G	2	0	0	0	0
8	J	2	0	0	0	0
9	A	1	0	0	0	0
9	J	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13519	0	12738	300	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 11.

All (300) 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:F:43:PRO:HD2	1:F:45:GLU:OE1	1.50	1.09
1:A:43:PRO:HG2	1:F:44:ARG:HH22	1.20	1.07
1:A:111:ARG:HE	1:A:128:GLU:HG3	1.20	1.05
4:I:95:SER:HB3	4:I:118:LEU:O	1.59	1.02
5:J:73:LYS:HG2	5:J:74:ASP:H	1.26	1.00
5:J:183:HIS:HA	7:J:263:CL:CL	1.99	0.99
1:A:43:PRO:HG2	1:F:44:ARG:NH2	1.78	0.98
5:J:115:ALA:O	5:J:118:THR:HG23	1.64	0.97
5:J:243:ARG:HG2	5:J:243:ARG:HH11	1.33	0.93
1:F:127:ASN:HD21	1:F:134:THR:HG23	1.30	0.92
4:D:40:PHE:HE1	5:E:118:THR:HG22	1.33	0.92
4:D:95:SER:HB3	4:D:118:LEU:O	1.70	0.88
4:D:40:PHE:CE1	5:E:118:THR:HG22	2.15	0.82
1:A:43:PRO:CG	1:F:44:ARG:NH2	2.44	0.80
1:F:35:ARG:CZ	2:G:53:ASP:HB2	2.12	0.79
5:E:73:LYS:HG2	5:E:74:ASP:H	1.46	0.78
1:F:187:THR:HB	1:F:272:LEU:HD21	1.64	0.78
5:E:57:GLN:NE2	5:E:110:TRP:HE1	1.83	0.77
5:E:73:LYS:HG2	5:E:74:ASP:OD1	1.84	0.77
5:J:96:LEU:HD23	7:J:266:CL:CL	2.22	0.76
5:J:73:LYS:CG	5:J:74:ASP:H	1.98	0.76
4:I:8:GLN:OE1	4:I:11:MET:CG	2.34	0.76
4:I:8:GLN:OE1	4:I:11:MET:HG3	1.85	0.75
1:F:35:ARG:NH2	2:G:54:LEU:O	2.20	0.75
5:E:45:ILE:HB	5:E:48:GLN:HG3	1.68	0.73
5:J:243:ARG:HG2	5:J:243:ARG:NH1	2.04	0.73
5:J:73:LYS:HG2	5:J:74:ASP:N	2.02	0.72
1:F:69:THR:HG23	5:J:57:GLN:HE22	1.53	0.72
4:D:124:ILE:HG21	4:D:151:ASP:HA	1.72	0.72
1:F:127:ASN:ND2	1:F:134:THR:HG23	2.05	0.71
2:G:33:SER:HB2	2:G:54:LEU:HD21	1.71	0.71
1:A:218:GLN:HG2	1:A:223:ASP:HA	1.73	0.70
2:B:83:ASN:HD22	2:B:84:HIS:H	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:SER:O	1:F:44:ARG:N	2.21	0.69
2:B:83:ASN:HD22	2:B:84:HIS:N	1.92	0.68
1:A:258:THR:HG22	1:A:273:ARG:HH12	1.57	0.68
1:F:35:ARG:NH1	2:G:53:ASP:HB2	2.08	0.68
4:D:79:ALA:HB3	7:D:2:CL:CL	2.31	0.67
5:J:96:LEU:CD2	5:J:96:LEU:H	2.08	0.67
1:F:144:GLN:O	1:F:148:GLU:HG2	1.95	0.67
1:A:82:ARG:NH2	1:A:89[B]:GLU:HG2	2.10	0.67
1:F:43:PRO:O	1:F:44:ARG:HB2	1.95	0.66
4:D:138:LYS:HG3	4:D:139:SER:H	1.61	0.66
1:A:69:THR:HG21	5:E:110:TRP:HZ2	1.61	0.66
5:E:233:LEU:HD23	5:E:246:PRO:HG2	1.77	0.65
5:J:183:HIS:HD2	5:J:184:SER:H	1.44	0.65
1:A:35:ARG:NH2	2:B:54:LEU:O	2.29	0.65
1:F:69:THR:HG23	5:J:57:GLN:NE2	2.12	0.65
4:I:95:SER:HA	4:I:96:ALA:HB3	1.79	0.64
4:D:95:SER:HA	4:D:96:ALA:HB3	1.78	0.64
5:J:19:VAL:HG23	5:J:91:ILE:HB	1.80	0.64
5:E:156:LYS:HG3	5:E:211:ARG:HH21	1.61	0.64
5:E:233:LEU:CD2	5:E:246:PRO:HG2	2.28	0.64
5:E:73:LYS:HG2	5:E:74:ASP:N	2.13	0.64
5:E:75:ARG:NH1	5:E:98:ASP:OD2	2.32	0.63
1:F:127:ASN:HD21	1:F:134:THR:CG2	2.07	0.63
5:J:239:TRP:HB2	5:J:245:LYS:HD3	1.80	0.63
5:J:73:LYS:NZ	5:J:75:ARG:HE	1.96	0.63
1:F:41:ALA:O	1:F:42:SER:HB2	1.99	0.62
1:F:43:PRO:O	1:F:44:ARG:CB	2.44	0.62
5:E:73:LYS:CG	5:E:74:ASP:H	2.12	0.62
1:A:43:PRO:HB3	1:F:43:PRO:HB3	1.81	0.62
1:F:207:GLY:HA2	1:F:240:THR:CG2	2.29	0.62
1:F:235:PRO:HG2	2:G:65:LEU:HD13	1.82	0.62
1:A:263:HIS:CD2	1:A:265:GLY:H	2.17	0.61
4:I:124:ILE:HG21	4:I:151:ASP:HA	1.80	0.61
1:A:207:GLY:HA2	1:A:240:THR:CG2	2.30	0.61
4:I:8:GLN:OE1	4:I:11:MET:SD	2.59	0.61
1:A:10:THR:HG23	1:A:96:GLN:HG2	1.82	0.61
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.83	0.60
1:F:69:THR:HG21	5:J:110:TRP:HZ2	1.66	0.60
1:A:20:PRO:HB2	1:A:22:PHE:CZ	2.35	0.60
2:B:7:ILE:HD12	2:B:82:VAL:HG21	1.82	0.60
1:F:207:GLY:HA2	1:F:240:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:HIS:CD2	1:F:265:GLY:H	2.19	0.60
1:F:41:ALA:O	1:F:42:SER:CB	2.49	0.60
4:I:139:SER:O	4:I:140:SER:CB	2.49	0.60
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.84	0.60
1:F:111:ARG:HE	1:F:128:GLU:HG3	1.66	0.59
1:A:111:ARG:NE	1:A:128:GLU:HG3	2.04	0.59
1:F:21:ARG:NE	1:F:23:ILE:HD11	2.18	0.59
4:D:95:SER:CA	4:D:96:ALA:HB3	2.32	0.59
4:I:74:LEU:HD11	4:I:83:ALA:HB1	1.85	0.59
5:E:22:TRP:NE1	5:E:86:ASP:OD1	2.30	0.59
1:F:19:GLU:OE1	1:F:75:ARG:NH2	2.36	0.59
5:E:11:LYS:HE3	5:E:13:ILE:CD1	2.33	0.59
1:F:187:THR:CB	1:F:272:LEU:HD21	2.33	0.58
4:I:40:PHE:HE1	5:J:118:THR:HG22	1.68	0.58
5:J:14:GLU:H	5:J:17:GLN:NE2	2.01	0.58
1:A:207:GLY:HA2	1:A:240:THR:HG21	1.84	0.58
2:G:83:ASN:HD22	2:G:84:HIS:N	2.03	0.57
5:J:138:PRO:HD3	5:J:246:PRO:HB3	1.86	0.57
1:A:273:ARG:HB3	1:A:273:ARG:NH1	2.19	0.57
5:E:115:ALA:O	5:E:118:THR:HG23	2.04	0.57
5:J:183:HIS:CD2	5:J:184:SER:H	2.23	0.57
5:J:178:ASN:ND2	5:J:223:HIS:H	2.03	0.57
1:F:71:THR:O	1:F:75:ARG:HG3	2.04	0.57
1:F:42:SER:C	1:F:44:ARG:H	2.08	0.57
4:I:95:SER:CA	4:I:96:ALA:HB3	2.35	0.57
5:J:173:LEU:HD21	5:J:226:CYS:SG	2.44	0.57
1:F:215:LEU:HD22	1:F:261:VAL:HG22	1.87	0.56
5:J:13:ILE:HG12	5:J:127:LEU:HD11	1.86	0.56
4:D:154:THR:HG21	4:D:205:PRO:HD3	1.86	0.56
1:A:42:SER:OG	1:A:45:GLU:HB3	2.05	0.56
1:F:119:ASP:HB3	2:G:0:MET:HA	1.87	0.56
5:J:161:CYS:HB2	5:J:175:TRP:CZ2	2.41	0.56
1:F:43:PRO:HD2	1:F:45:GLU:CD	2.23	0.56
4:D:4:ILE:HD11	4:D:102:MET:HB2	1.87	0.55
1:F:42:SER:HB3	1:F:45:GLU:OE1	2.06	0.55
5:E:19:VAL:HG23	5:E:91:ILE:HB	1.89	0.55
5:E:143:VAL:HG23	5:E:253:ALA:HB3	1.87	0.55
1:A:82:ARG:CZ	1:A:89[B]:GLU:HG2	2.36	0.55
5:E:71:LEU:HD22	5:E:76:PHE:HB3	1.88	0.54
4:I:56:GLN:HB2	4:I:74:LEU:HD23	1.90	0.54
1:A:42:SER:CB	1:A:45:GLU:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.90	0.53
1:A:71:THR:O	1:A:75:ARG:HG3	2.09	0.53
1:F:40:ALA:O	1:F:41:ALA:HB3	2.07	0.53
5:J:96:LEU:HA	5:J:129:VAL:HB	1.89	0.53
5:J:146:PRO:HD2	5:J:217:TRP:CZ2	2.44	0.53
1:A:35:ARG:O	1:A:46:GLU:HG2	2.08	0.52
5:J:96:LEU:HD22	5:J:96:LEU:H	1.73	0.52
5:E:143:VAL:HG23	5:E:253:ALA:CB	2.40	0.52
1:F:20:PRO:HB2	1:F:22:PHE:CZ	2.44	0.52
2:G:49:VAL:HG12	2:G:68:THR:HB	1.92	0.52
1:A:44:ARG:O	1:A:48:ARG:NH2	2.44	0.52
4:I:164:VAL:HA	4:I:188:SER:OG	2.10	0.52
4:D:174:MET:O	4:D:176:SER:N	2.44	0.51
1:A:89[A]:GLU:CD	1:A:89[A]:GLU:H	2.12	0.51
5:J:15:LYS:O	5:J:16:ARG:HB2	2.10	0.51
1:A:81:LEU:HD21	3:C:9:LEU:HD22	1.91	0.51
4:D:7:THR:O	4:D:8:GLN:HB2	2.10	0.51
1:A:69:THR:HG21	5:E:110:TRP:CZ2	2.42	0.51
4:D:170:CYS:HB3	5:E:209:ARG:HH12	1.75	0.51
5:J:13:ILE:HD13	5:J:19:VAL:HG22	1.92	0.51
1:A:35:ARG:CZ	2:B:53:ASP:HB3	2.41	0.51
1:F:190:THR:OG1	1:F:192:HIS:HE1	1.94	0.51
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.41	0.51
4:I:29:ASP:OD2	4:I:106:THR:HB	2.11	0.51
1:F:35:ARG:NH1	2:G:53:ASP:CB	2.73	0.51
4:D:74:LEU:HD11	4:D:83:ALA:HB1	1.93	0.50
4:I:125:GLN:O	4:I:126:ASN:HB2	2.11	0.50
1:A:219:ARG:HD3	1:A:257:TYR:CZ	2.45	0.50
5:J:243:ARG:NH1	5:J:243:ARG:CG	2.73	0.50
5:J:199:LEU:HD12	5:J:199:LEU:H	1.76	0.50
5:J:73:LYS:CG	5:J:74:ASP:N	2.68	0.50
1:A:40:ALA:O	1:A:41:ALA:HB3	2.11	0.50
1:F:172:LEU:HD23	1:F:179:LEU:HD23	1.94	0.50
5:J:95:LYS:HB3	7:J:266:CL:CL	2.48	0.50
4:D:209:PHE:HE1	4:D:211:PRO:HB3	1.76	0.50
5:E:11:LYS:HE3	5:E:13:ILE:HD11	1.94	0.50
4:I:197:ASN:HA	4:I:200:ASN:ND2	2.27	0.50
4:D:190:LYS:HG3	4:D:192:ASP:OD2	2.12	0.49
4:D:139:SER:O	4:D:140:SER:CB	2.61	0.49
5:J:178:ASN:HD22	5:J:223:HIS:H	1.59	0.49
5:J:96:LEU:HD23	5:J:96:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.94	0.49
5:E:138:PRO:HD3	5:E:246:PRO:HB3	1.95	0.49
4:I:137:SER:O	4:I:138:LYS:HB2	2.13	0.49
5:J:73:LYS:HZ3	5:J:75:ARG:HE	1.61	0.49
1:A:210:PRO:O	1:A:263:HIS:HE1	1.96	0.49
1:A:42:SER:OG	1:A:45:GLU:CB	2.61	0.49
5:E:14:GLU:H	5:E:17:GLN:NE2	2.11	0.49
4:I:132:TYR:CE1	5:J:150:GLU:HG3	2.48	0.49
1:A:31:THR:HG23	1:A:239:ARG:HH21	1.77	0.49
1:A:32:GLN:O	1:A:239:ARG:NH2	2.45	0.48
4:D:46:SER:O	4:D:47:SER:OG	2.30	0.48
5:E:73:LYS:HE2	5:E:74:ASP:OD1	2.13	0.48
5:E:161:CYS:HB2	5:E:175:TRP:CZ2	2.47	0.48
4:D:41:TRP:HB2	4:D:54:ILE:HG22	1.95	0.48
1:A:41:ALA:O	1:A:42:SER:CB	2.62	0.48
5:E:237:ASP:O	5:E:245:LYS:NZ	2.35	0.48
1:A:42:SER:HB3	1:A:45:GLU:HB3	1.95	0.48
5:E:75:ARG:HH12	5:E:98:ASP:CG	2.17	0.48
5:E:146:PRO:HD2	5:E:217:TRP:CZ2	2.49	0.47
5:J:234:SER:O	5:J:245:LYS:HE3	2.14	0.47
4:D:96:ALA:HB1	4:D:98:TYR:CE2	2.49	0.47
5:J:75:ARG:NH1	5:J:98:ASP:OD2	2.48	0.47
1:F:239:ARG:HH11	1:F:239:ARG:HB2	1.80	0.47
5:J:136:VAL:HG12	5:J:246:PRO:HG2	1.97	0.47
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.48	0.47
4:D:161:ASP:OD1	4:D:161:ASP:N	2.47	0.47
1:F:123:TYR:CE2	3:H:9:LEU:HD23	2.48	0.47
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.80	0.47
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.80	0.47
1:A:22:PHE:HB2	1:A:38:SER:HB3	1.97	0.47
4:I:174:MET:O	4:I:176:SER:N	2.47	0.47
1:F:69:THR:HG21	5:J:110:TRP:CZ2	2.47	0.46
1:A:187:THR:HG21	1:A:261:VAL:HG21	1.96	0.46
1:A:273:ARG:HB3	1:A:273:ARG:HH11	1.80	0.46
1:F:14:ARG:NH1	1:F:21:ARG:HB2	2.30	0.46
1:A:238:ASP:OD2	1:A:240:THR:HG22	2.15	0.46
5:E:146:PRO:HG2	5:E:157:ALA:HB1	1.97	0.46
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.50	0.46
5:J:217:TRP:CZ2	5:J:258:ARG:HG3	2.50	0.46
5:E:96:LEU:HA	5:E:129:VAL:HB	1.98	0.46
4:I:139:SER:O	4:I:140:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:245:LYS:HG3	5:E:246:PRO:HD2	1.98	0.46
5:E:73:LYS:CE	5:E:74:ASP:OD1	2.63	0.46
1:F:185:PRO:HD2	1:F:266:LEU:HD13	1.98	0.46
4:I:4:ILE:HD11	4:I:102:MET:HB2	1.98	0.46
4:I:151:ASP:OD2	4:I:153:GLN:HG2	2.16	0.46
4:D:27:THR:HG21	4:D:32:TYR:CE2	2.51	0.46
1:A:178:THR:O	1:A:181:ARG:HG2	2.16	0.45
4:D:13:VAL:HG21	4:D:19:VAL:HG22	1.98	0.45
4:D:47:SER:OG	4:D:47:SER:O	2.33	0.45
4:I:101:ALA:HA	4:I:111:TYR:O	2.15	0.45
1:F:32:GLN:HE22	1:F:47:PRO:HB2	1.80	0.45
1:A:19:GLU:OE1	1:A:75:ARG:NH2	2.50	0.45
1:F:121:LYS:HB3	2:G:1:ILE:HD12	1.99	0.45
1:F:133:TRP:HB2	1:F:144:GLN:HE21	1.81	0.45
1:F:51:TRP:HA	1:F:54:GLN:HG2	1.99	0.45
1:A:147:TRP:CD1	1:A:152:VAL:HG21	2.51	0.45
5:E:73:LYS:CG	5:E:74:ASP:N	2.77	0.45
1:F:123:TYR:CZ	1:F:140:ALA:HA	2.51	0.45
2:G:39:LEU:HB3	2:G:46:ILE:HD12	1.99	0.45
5:E:239:TRP:CZ2	5:E:246:PRO:HD3	2.52	0.44
5:J:73:LYS:HG2	5:J:74:ASP:OD2	2.16	0.44
4:D:138:LYS:CG	4:D:139:SER:H	2.28	0.44
4:D:170:CYS:CB	5:E:209:ARG:HH12	2.29	0.44
5:E:227:GLN:HG3	5:E:250:ILE:HG23	1.99	0.44
5:J:71:LEU:O	5:J:73:LYS:N	2.50	0.44
1:A:67:PHE:O	1:A:71:THR:HG23	2.18	0.44
5:J:22:TRP:HE1	5:J:86:ASP:CG	2.21	0.44
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.99	0.44
2:B:83:ASN:ND2	2:B:84:HIS:N	2.63	0.44
4:D:101:ALA:HA	4:D:111:TYR:O	2.17	0.44
1:F:178:THR:O	1:F:181:ARG:HG3	2.17	0.44
5:J:146:PRO:CG	5:J:157:ALA:HB1	2.47	0.44
1:A:31:THR:CG2	1:A:239:ARG:HH21	2.31	0.44
5:E:12:ILE:HD12	5:E:232:GLY:HA2	1.99	0.44
5:J:196:GLN:HB2	5:J:199:LEU:HD13	1.99	0.44
1:A:207:GLY:HA2	1:A:240:THR:HG23	2.00	0.43
2:B:59:ASP:O	2:B:60:TRP:HB2	2.18	0.43
5:E:15:LYS:O	5:E:16:ARG:HB2	2.18	0.43
5:J:54:ILE:HG13	5:J:68:ASP:HB3	1.99	0.43
4:D:139:SER:O	4:D:140:SER:HB2	2.17	0.43
1:F:190:THR:OG1	1:F:192:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:116:TYR:HB2	1:F:124:ILE:HG22	1.99	0.43
4:I:7:THR:O	4:I:8:GLN:HB2	2.18	0.43
1:A:65:GLN:O	1:A:69:THR:HB	2.19	0.43
4:I:127:PRO:HB3	4:I:151:ASP:HB3	2.00	0.43
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.42
1:F:210:PRO:O	1:F:263:HIS:HE1	2.02	0.42
5:J:22:TRP:CH2	5:J:24:ASN:HB2	2.54	0.42
1:A:224:GLN:O	1:A:225:THR:CB	2.67	0.42
3:H:5:ARG:HD2	9:J:268:HOH:O	2.18	0.42
4:D:103:ARG:NH1	4:D:105:ASP:OD1	2.45	0.42
1:F:51:TRP:HA	1:F:54:GLN:HE21	1.84	0.42
4:D:42:TYR:CE2	4:D:52:PHE:HB2	2.54	0.42
5:J:182:VAL:O	5:J:182:VAL:HG13	2.19	0.42
1:F:46:GLU:O	1:F:48:ARG:N	2.53	0.42
4:I:27:THR:HG21	4:I:32:TYR:CE1	2.54	0.42
5:J:54:ILE:HG12	5:J:55:GLN:N	2.35	0.42
4:I:45:PRO:HA	4:I:96:ALA:H	1.85	0.42
4:D:189:ASN:OD1	4:D:189:ASN:N	2.43	0.42
4:D:29:ASP:OD2	4:D:106:THR:HB	2.19	0.42
2:G:71:THR:HA	2:G:72:PRO:HD2	1.94	0.42
5:J:146:PRO:HG2	5:J:157:ALA:HB1	2.02	0.42
5:J:143:VAL:HG23	5:J:253:ALA:HB3	2.00	0.42
5:E:13:ILE:HG22	5:E:129:VAL:HG13	2.02	0.41
1:A:81:LEU:HA	1:A:81:LEU:HD13	1.86	0.41
5:E:22:TRP:CH2	5:E:24:ASN:HB2	2.54	0.41
5:E:2:MET:HB3	5:E:3:GLY:H	1.65	0.41
1:F:35:ARG:NH1	1:F:37:ASP:OD2	2.54	0.41
1:F:238:ASP:OD2	1:F:240:THR:HB	2.20	0.41
1:F:65:GLN:O	1:F:69:THR:HB	2.21	0.41
4:D:15:GLU:HG3	4:D:122:PRO:HA	2.03	0.41
1:F:9:ASP:HB2	1:F:97:SER:HB3	2.02	0.41
5:J:22:TRP:NE1	5:J:86:ASP:OD1	2.52	0.41
5:J:227:GLN:HG3	5:J:250:ILE:HG23	2.02	0.41
1:A:172:LEU:HD23	1:A:179:LEU:HD23	2.03	0.41
1:A:236:ALA:HB3	1:A:240:THR:HG22	2.01	0.41
1:F:236:ALA:HB3	1:F:240:THR:HG22	2.02	0.41
5:E:191:GLN:HA	5:E:192:PRO:HD3	1.91	0.41
4:D:44:GLN:NE2	5:E:44:GLN:OE1	2.46	0.41
5:J:73:LYS:HZ1	5:J:75:ARG:HE	1.67	0.41
1:A:81:LEU:HD21	3:C:9:LEU:CD2	2.51	0.41
2:B:57:SER:HB2	2:B:59:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:187:CYS:O	5:E:208:SER:HA	2.21	0.41
1:A:62:ARG:HG2	4:D:105:ASP:O	2.21	0.41
5:E:26:ILE:HB	5:E:29:HIS:CD2	2.55	0.41
5:J:239:TRP:CB	5:J:245:LYS:HD3	2.49	0.41
5:J:96:LEU:CD2	5:J:96:LEU:N	2.77	0.41
1:A:98:MET:HE2	1:A:98:MET:HB2	1.96	0.41
2:G:30:PHE:CE2	2:G:62:PHE:HB2	2.55	0.41
1:A:157:ARG:O	1:A:161:GLU:HG3	2.20	0.40
4:D:190:LYS:HA	4:D:190:LYS:HD2	1.83	0.40
4:I:32:TYR:CD2	4:I:58:SER:HB3	2.56	0.40
5:J:128:THR:OG1	5:J:170:HIS:CE1	2.74	0.40
4:I:167:THR:OG1	4:I:168:ASP:N	2.55	0.40
4:D:132:TYR:HB3	5:E:147:SER:OG	2.21	0.40
4:I:196:ALA:HA	4:I:210:PHE:CE2	2.57	0.40
4:D:190:LYS:HE3	4:D:191:SER:H	1.86	0.40
4:D:54:ILE:HG13	4:D:55:TYR:N	2.36	0.40
5:E:239:TRP:HB2	5:E:245:LYS:HD3	2.04	0.40
5:J:191:GLN:HA	5:J:192:PRO:HD3	1.90	0.40
5:J:199:LEU:HD12	5:J:199:LEU:N	2.36	0.40
1:F:40:ALA:O	1:F:41:ALA:CB	2.70	0.40
5:J:192:PRO:HB2	5:J:204:TYR:CD1	2.57	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	277/277 (100%)	263 (95%)	8 (3%)	6 (2%)	6	22
1	F	274/277 (99%)	260 (95%)	9 (3%)	5 (2%)	8	28
2	B	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
2	G	98/100 (98%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	200/202 (99%)	174 (87%)	19 (10%)	7 (4%)	3	12
4	I	202/202 (100%)	178 (88%)	16 (8%)	8 (4%)	3	9
5	E	245/247 (99%)	225 (92%)	14 (6%)	6 (2%)	6	20
5	J	246/247 (100%)	224 (91%)	17 (7%)	5 (2%)	7	24
All	All	1655/1670 (99%)	1528 (92%)	90 (5%)	37 (2%)	6	22

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
4	D	140	SER
4	D	175	ARG
5	E	73	LYS
5	E	93	PRO
1	F	40	ALA
1	F	47	PRO
4	I	140	SER
4	I	175	ARG
5	J	73	LYS
5	J	93	PRO
1	A	47	PRO
1	A	225	THR
4	D	138	LYS
5	E	183	HIS
1	F	41	ALA
4	I	138	LYS
5	E	72	PRO
5	E	85	VAL
5	E	153	HIS
1	F	43	PRO
4	I	167	THR
5	J	72	PRO
5	J	85	VAL
5	J	153	HIS
1	A	41	ALA
1	A	86	ASN
4	D	8	GLN
4	D	96	ALA

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Mol	Chain	Res	Type
4	D	167	THR
4	I	8	GLN
4	I	96	ALA
4	D	126	ASN
1	F	42	SER
4	I	48	GLY
4	I	126	ASN
1	A	42	SER

### 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	238/236 (101%)	213 (90%)	25 (10%)	7	20
1	F	235/236 (100%)	213 (91%)	22 (9%)	8	26
2	B	96/95 (101%)	87 (91%)	9 (9%)	8	26
2	G	95/95 (100%)	87 (92%)	8 (8%)	11	31
3	C	6/6 (100%)	6 (100%)	0	100	100
3	H	6/6 (100%)	6 (100%)	0	100	100
4	D	179/179 (100%)	161 (90%)	18 (10%)	7	22
4	I	181/179 (101%)	157 (87%)	24 (13%)	4	12
5	E	213/213 (100%)	194 (91%)	19 (9%)	9	28
5	J	214/213 (100%)	193 (90%)	21 (10%)	8	24
All	All	1463/1458 (100%)	1317 (90%)	146 (10%)	7	22

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	10	THR
1	A	12	MET
1	A	69	THR
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	89[A]	GLU
1	A	89[B]	GLU
1	A	151	ARG
1	A	166	GLU
1	A	169	ARG
1	A	179	LEU
1	A	186	LYS
1	A	206	LEU
1	A	215	LEU
1	A	216	THR
1	A	223	ASP
1	A	226	GLN
1	A	230	LEU
1	A	240	THR
1	A	254	GLU
1	A	262	GLN
1	A	268	LYS
1	A	271	THR
1	A	273	ARG
1	A	277	SER
2	B	4	THR
2	B	50	GLU
2	B	53	ASP
2	B	70	PHE
2	B	75	LYS
2	B	81	ARG
2	B	83	ASN
2	B	94	LYS
2	B	97	ARG
4	D	19	VAL
4	D	39	LEU
4	D	60	ASP
4	D	73	SER
4	D	74	LEU
4	D	95	SER
4	D	97	MET
4	D	104	GLU
4	D	106	THR
4	D	116	THR
4	D	119	THR
4	D	123	ASN
4	D	124	ILE

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Mol	Chain	Res	Type
4	D	128	ASP
4	D	136	ASP
4	D	142	LYS
4	D	181	SER
4	D	190	LYS
5	E	13	ILE
5	E	19	VAL
5	E	29	HIS
5	E	57	GLN
5	E	59	ASN
5	E	73	LYS
5	E	79	GLU
5	E	81	LEU
5	E	104	CYS
5	E	141	VAL
5	E	148	GLU
5	E	154	THR
5	E	170	HIS
5	E	180	LYS
5	E	187	CYS
5	E	196	GLN
5	E	209	ARG
5	E	212	VAL
5	E	233	LEU
1	F	25	VAL
1	F	32	GLN
1	F	34	VAL
1	F	46	GLU
1	F	69	THR
1	F	81	LEU
1	F	86	ASN
1	F	148	GLU
1	F	151	ARG
1	F	176	LYS
1	F	180	GLU
1	F	181	ARG
1	F	186	LYS
1	F	206	LEU
1	F	216	THR
1	F	223	ASP
1	F	230	LEU
1	F	240	THR

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Mol	Chain	Res	Type
1	F	254	GLU
1	F	266	LEU
1	F	272	LEU
1	F	273	ARG
2	G	4	THR
2	G	7	ILE
2	G	47	GLU
2	G	48	LYS
2	G	70	PHE
2	G	83	ASN
2	G	89	GLN
2	G	99	MET
4	I	11	MET
4	I	19	VAL
4	I	24	THR
4	I	28	SER
4	I	60	ASP
4	I	80	ARG
4	I	95	SER
4	I	97	MET
4	I	106	THR
4	I	119	THR
4	I	123	ASN
4	I	124	ILE
4	I	136	ASP
4	I	143	SER
4	I	153	GLN
4	I	157	SER
4	I	160	LYS
4	I	161	ASP
4	I	170	CYS
4	I	181	SER
4	I	183	SER
4	I	189	ASN
4	I	191	SER
4	I	207	ASP
5	J	2	MET
5	J	19	VAL
5	J	29	HIS
5	J	71	LEU
5	J	73	LYS
5	J	92	GLN

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Mol	Chain	Res	Type
5	J	96	LEU
5	J	141	VAL
5	J	147	SER
5	J	170	HIS
5	J	178	ASN
5	J	181	GLU
5	J	183	HIS
5	J	196	GLN
5	J	201	ASP
5	J	215	THR
5	J	233	LEU
5	J	235	GLU
5	J	238	GLU
5	J	243	ARG
5	J	260	ASP

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	54	GLN
1	A	127	ASN
1	A	174	ASN
1	A	192	HIS
1	A	262	GLN
1	A	263	HIS
2	B	83	ASN
2	B	89	GLN
4	D	201	ASN
5	E	17	GLN
5	E	29	HIS
5	E	57	GLN
5	E	153	HIS
5	E	170	HIS
5	E	249	GLN
1	F	32	GLN
1	F	54	GLN
1	F	86	ASN
1	F	127	ASN
1	F	144	GLN
1	F	174	ASN
1	F	192	HIS
1	F	262	GLN

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Mol	Chain	Res	Type
1	F	263	HIS
2	G	83	ASN
4	I	123	ASN
4	I	200	ASN
5	J	17	GLN
5	J	29	HIS
5	J	92	GLN
5	J	170	HIS
5	J	178	ASN
5	J	183	HIS
5	J	200	ASN
5	J	249	GLN

### 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 31 ligands modelled in this entry, 31 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	277/277 (100%)	0.19	16 (5%) 23 15	17, 30, 54, 66	18 (6%)
1	F	276/277 (99%)	0.13	10 (3%) 42 32	17, 30, 53, 66	19 (6%)
2	B	100/100 (100%)	-0.24	0 100 100	16, 26, 40, 46	4 (4%)
2	G	100/100 (100%)	-0.33	1 (1%) 82 77	16, 26, 40, 45	6 (6%)
3	C	9/9 (100%)	-0.42	0 100 100	22, 23, 28, 29	0
3	H	9/9 (100%)	-0.37	0 100 100	19, 21, 24, 25	0
4	D	202/202 (100%)	0.77	33 (16%) 1 1	24, 58, 84, 91	2 (0%)
4	I	202/202 (100%)	0.68	18 (8%) 9 5	24, 58, 84, 90	6 (2%)
5	E	247/247 (100%)	0.11	6 (2%) 59 49	15, 28, 66, 77	7 (2%)
5	J	247/247 (100%)	0.10	8 (3%) 47 37	15, 28, 66, 77	6 (2%)
All	All	1669/1670 (99%)	0.22	92 (5%) 25 16	15, 34, 79, 91	68 (4%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	42	SER	5.8
1	F	43	PRO	5.6
1	A	41	ALA	5.2
1	F	41	ALA	4.8
4	I	192	ASP	4.7
4	D	159	SER	4.7
1	A	221	GLY	4.5
4	D	160	LYS	4.4
4	D	208	THR	4.3
4	I	139	SER	4.2
4	D	162	SER	4.2
1	A	43	PRO	4.2
1	A	277	SER	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	D	191	SER	4.1
1	A	45	GLU	4.0
4	D	212	SER	3.9
4	D	197	ASN	3.9
4	D	161	ASP	3.8
1	A	223	ASP	3.8
4	D	200	ASN	3.8
1	A	42	SER	3.7
5	J	259	ALA	3.6
1	A	195	SER	3.4
4	D	193	PHE	3.3
4	D	141	ASP	3.3
1	A	220	ASP	3.2
1	F	196	ASP	3.2
4	D	178	ASP	3.2
4	D	150	PHE	3.2
4	I	162	SER	3.2
4	D	147	PHE	3.1
5	J	260	ASP	3.1
5	E	200	ASN	3.0
1	F	195	SER	3.0
4	I	8	GLN	3.0
4	I	125	GLN	2.9
4	D	135	ARG	2.9
2	G	0	MET	2.9
4	D	137	SER	2.8
1	F	44	ARG	2.8
4	D	143	SER	2.8
4	I	160	LYS	2.7
4	D	163	ASP	2.7
1	A	197	HIS	2.7
4	I	130	ALA	2.7
4	I	195	CYS	2.7
1	F	40	ALA	2.6
4	I	147	PHE	2.6
4	D	195	CYS	2.6
1	A	40	ALA	2.6
4	I	202	SER	2.6
5	E	257	GLY	2.6
1	F	45	GLU	2.6
5	J	200	ASN	2.6
5	J	220	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	190	LYS	2.5
4	I	126	ASN	2.5
5	E	199	LEU	2.5
1	A	194	ILE	2.5
4	D	121	ILE	2.5
4	D	142	LYS	2.5
4	I	133	GLN	2.4
4	I	143	SER	2.4
1	F	197	HIS	2.4
5	J	201	ASP	2.4
4	I	191	SER	2.4
4	D	199	PHE	2.4
4	I	145	CYS	2.3
4	I	142	LYS	2.3
4	D	127	PRO	2.3
4	I	187	TRP	2.2
5	E	213	SER	2.2
4	D	173	ASP	2.2
4	D	140	SER	2.2
1	A	44	ARG	2.2
1	F	194	ILE	2.2
1	A	196	ASP	2.2
5	E	260	ASP	2.2
4	D	155	ASN	2.1
1	A	50	PRO	2.1
4	D	144	VAL	2.1
1	A	218	GLN	2.1
4	D	130	ALA	2.1
4	D	138	LYS	2.1
4	D	139	SER	2.1
5	J	193	LEU	2.1
5	E	149	ALA	2.1
5	J	257	GLY	2.1
4	D	203	ILE	2.0
5	J	217	TRP	2.0
4	I	75	ASN	2.0
4	D	189	ASN	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors(Å <sup>2</sup> )	Q<0.9
6	CD	F	278	1/1	0.74	0.14	46,46,46,46	0
6	CD	E	261	1/1	0.76	0.11	134,134,134,134	0
8	NA	A	282	1/1	0.79	0.25	52,52,52,52	0
6	CD	B	101	1/1	0.84	0.21	127,127,127,127	0
8	NA	D	213	1/1	0.85	0.25	36,36,36,36	1
8	NA	G	104	1/1	0.88	0.38	35,35,35,35	0
6	CD	G	101	1/1	0.90	0.21	121,121,121,121	0
8	NA	J	265	1/1	0.91	0.10	50,50,50,50	0
6	CD	B	100	1/1	0.92	0.11	34,34,34,34	0
7	CL	A	280	1/1	0.92	0.25	37,37,37,37	0
7	CL	J	266	1/1	0.92	0.32	60,60,60,60	0
7	CL	J	263	1/1	0.92	0.14	55,55,55,55	0
7	CL	E	264	1/1	0.93	0.19	57,57,57,57	0
8	NA	J	262	1/1	0.93	0.37	25,25,25,25	0
7	CL	B	102	1/1	0.93	0.19	55,55,55,55	0
6	CD	E	262	1/1	0.93	0.17	139,139,139,139	0
8	NA	B	104	1/1	0.94	0.11	23,23,23,23	0
7	CL	F	279	1/1	0.94	0.18	34,34,34,34	0
7	CL	J	264	1/1	0.94	0.08	49,49,49,49	0
8	NA	G	103	1/1	0.94	0.28	27,27,27,27	0
7	CL	D	2	1/1	0.95	0.13	39,39,39,39	0
6	CD	A	278	1/1	0.95	0.12	45,45,45,45	0
8	NA	E	263	1/1	0.96	0.28	23,23,23,23	0
6	CD	J	261	1/1	0.96	0.18	122,122,122,122	0
7	CL	A	283	1/1	0.97	0.13	36,36,36,36	0
8	NA	A	281	1/1	0.98	0.30	21,21,21,21	0
6	CD	I	213	1/1	0.98	0.14	52,52,52,52	1
7	CL	A	279	1/1	0.98	0.15	27,27,27,27	0
8	NA	B	103	1/1	0.98	0.45	17,17,17,17	0
7	CL	G	102	1/1	0.98	0.26	33,33,33,33	0
6	CD	G	100	1/1	1.00	0.11	35,35,35,35	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.