



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:18 PM GMT

PDB ID : 1JNH  
Title : Crystal Structure of Fab-Estradiol Complexes  
Authors : Monnet, C.; Bettsworth, F.; Stura, E.A.; Le Du, M.-H.; Menez, R.; Derrien, L.; Zinn-Justin, S.; Gilquin, B.; Sibai, G.; Battail-Poirot, N.; Jolivet, M.; Menez, A.; Arnaud, M.; Ducancel, F.; Charbonnier, J.B.  
Deposited on : 2001-07-24  
Resolution : 2.85 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

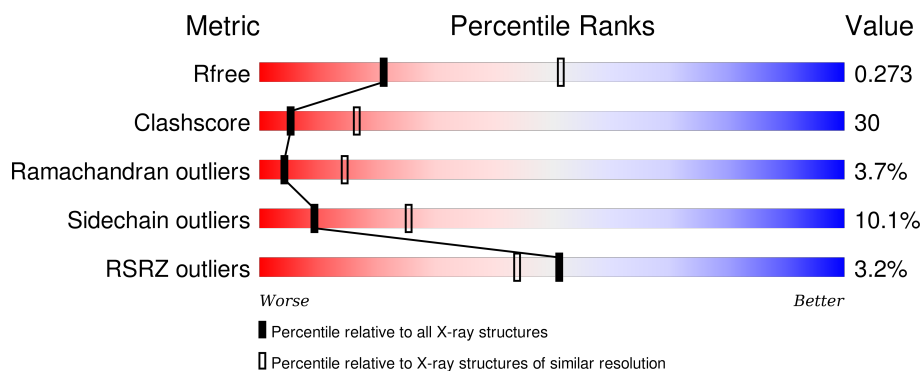
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	212	<div> <div>2%</div> <div>55%</div> <div>39%</div> <div>...</div> </div>
1	C	212	<div> <div>6%</div> <div>46%</div> <div>47%</div> <div>...</div> </div>
1	E	212	<div> <div>15%</div> <div>42%</div> <div>48%</div> <div>8%</div> <div>.</div> </div>
1	G	212	<div> <div>%</div> <div>52%</div> <div>40%</div> <div>5%</div> <div>.</div> </div>
2	B	218	<div> <div>48%</div> <div>44%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	218	
2	F	218	
2	H	218	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ECO	H	354	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12882 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 MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN LAMBDA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	C	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	E	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			
1	G	208	Total	C	N	O	S	0	0	0
			1567	979	262	321	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	-	SEE REMARK 999	UNP P01843
A	211	ALA	-	SEE REMARK 999	UNP P01843
C	210	ALA	-	SEE REMARK 999	UNP P01843
C	211	ALA	-	SEE REMARK 999	UNP P01843
E	210	ALA	-	SEE REMARK 999	UNP P01843
E	211	ALA	-	SEE REMARK 999	UNP P01843
G	210	ALA	-	SEE REMARK 999	UNP P01843
G	211	ALA	-	SEE REMARK 999	UNP P01843

- Molecule 2 is a protein called MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN GAMMA-1 CHAIN.

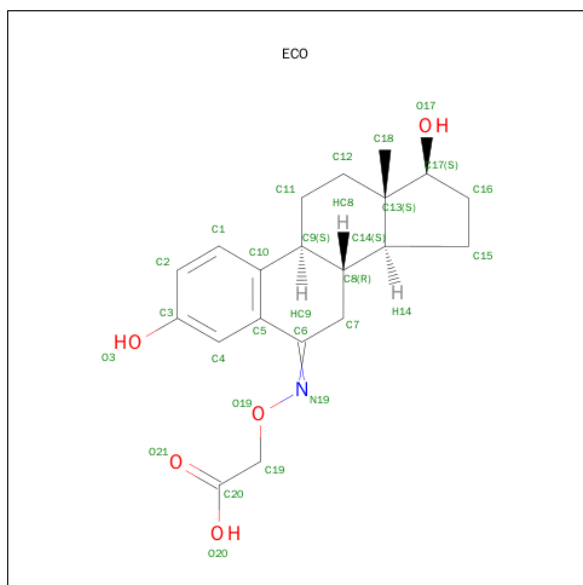
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			
2	D	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			
2	F	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1614	1021	267	319	7			

- Molecule 3 is ESTRADIOL-6 CARBOXYL-METHYL-OXIME (three-letter code: ECO) (formula:  $C_{20}H_{25}NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			26	20	1	5		
3	D	1	Total	C	N	O	0	0
			26	20	1	5		
3	F	1	Total	C	N	O	0	0
			26	20	1	5		
3	H	1	Total	C	N	O	0	0
			26	20	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	6	Total	O	0	0
			6	6		
4	C	3	Total	O	0	0
			3	3		
4	D	10	Total	O	0	0
			10	10		

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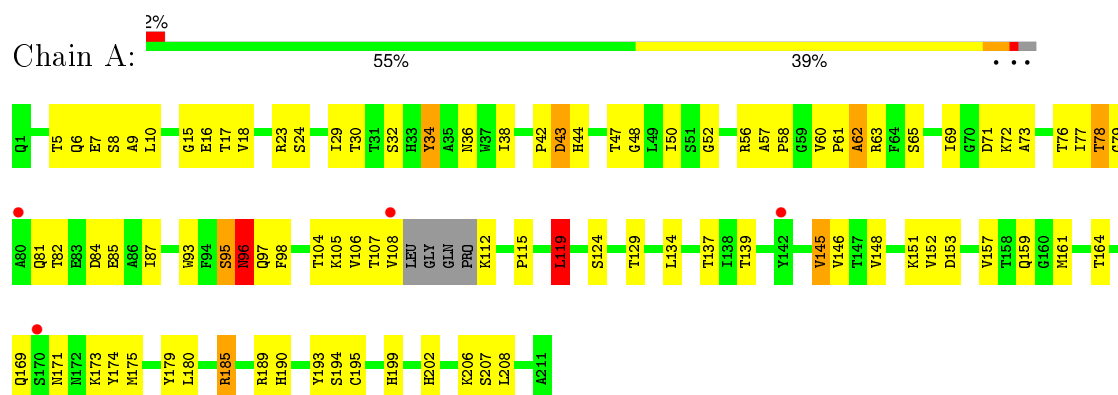
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	6	Total 6	O 6	0	0
4	F	4	Total 4	O 4	0	0
4	G	8	Total 8	O 8	0	0
4	H	10	Total 10	O 10	0	0

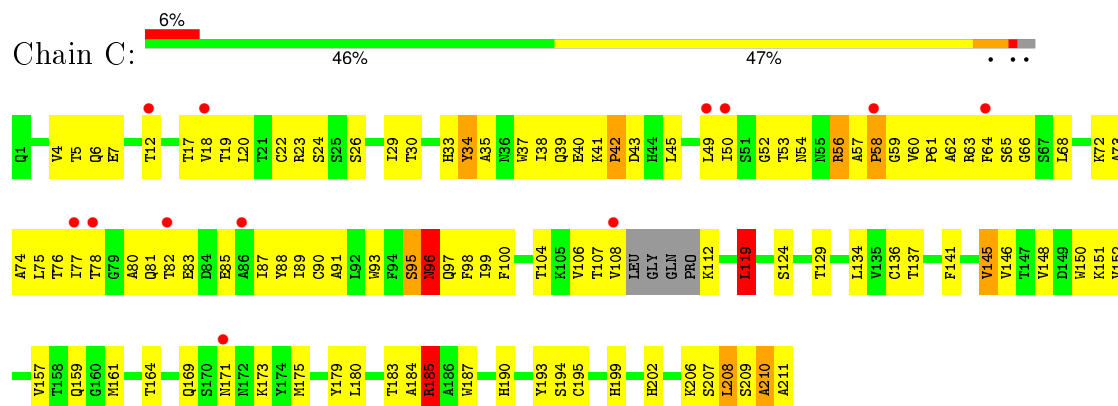
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

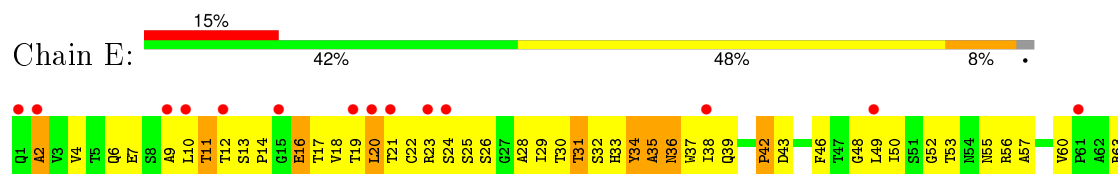
#### • Molecule 1: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN LAMBDA CHAIN

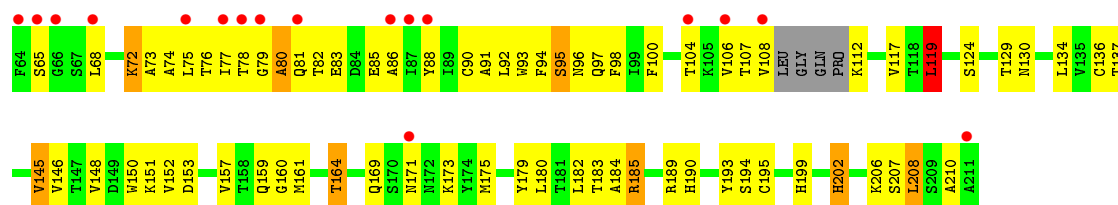


#### • Molecule 1: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN LAMBDA CHAIN

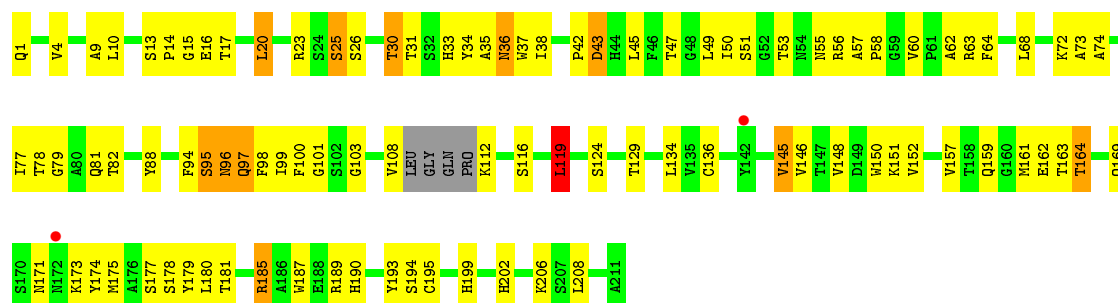


#### • Molecule 1: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN LAMBDA CHAIN

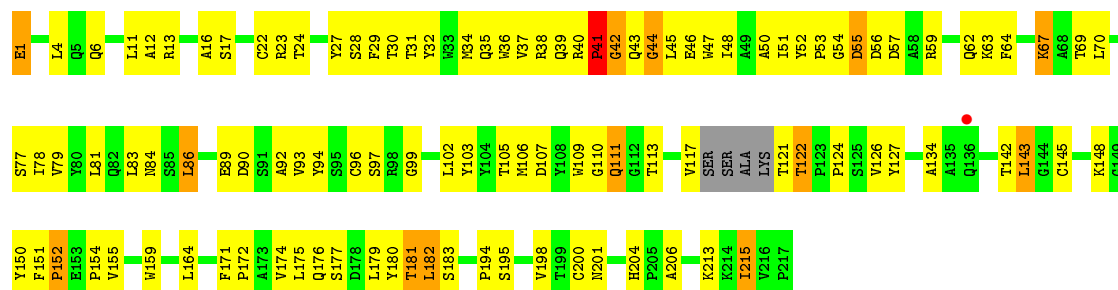




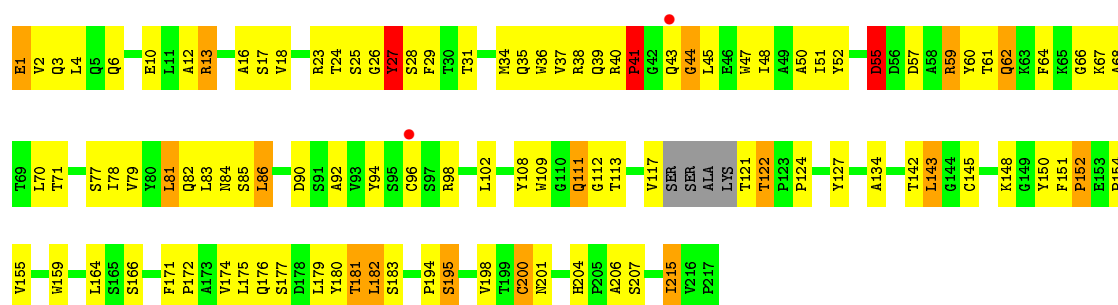
• Molecule 1: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN LAMBDA CHAIN



• Molecule 2: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN GAMMA-1 CHAIN



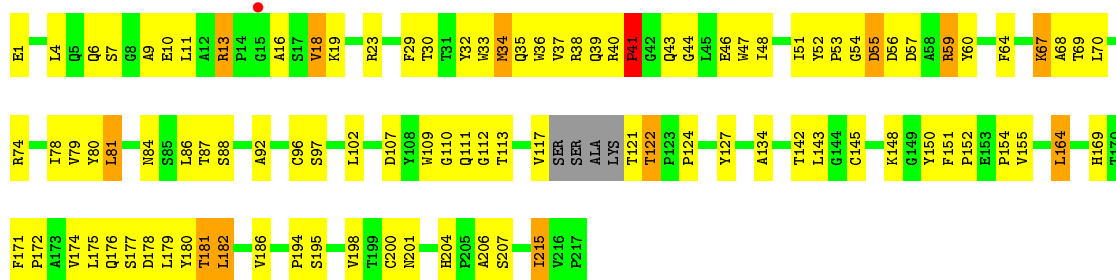
• Molecule 2: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN GAMMA-1 CHAIN





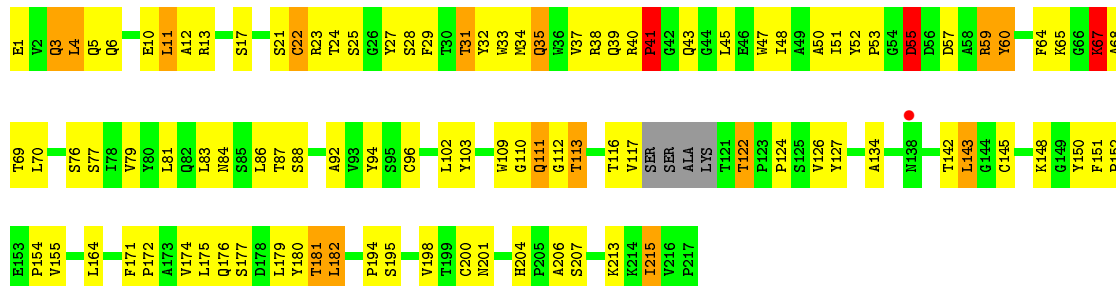
• Molecule 2: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN GAMMA-1 CHAIN

Chain F:  52% 40% 6% .



• Molecule 2: MONOCLONAL ANTI-ESTRADIOL 10G6D6 IMMUNOGLOBULIN GAMMA-1 CHAIN

Chain H:  51% 39% 7% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.20Å 192.90Å 71.12Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85 39.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	83.3 (40.00-2.85) 85.8 (39.73-2.60)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.198 , 0.253 0.221 , 0.273	Depositor DCC
$R_{free}$ test set	2139 reflections (5.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 71.3	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.053 for h,-k,-l 0.016 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 54098 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	0/1601	0.70	1/2185 (0.0%)
1	C	0.42	0/1601	0.69	1/2185 (0.0%)
1	E	0.43	0/1601	0.68	1/2185 (0.0%)
1	G	0.44	0/1601	0.70	1/2185 (0.0%)
2	B	0.41	0/1656	0.71	0/2266
2	D	0.44	0/1656	0.69	0/2266
2	F	0.40	0/1656	0.67	0/2266
2	H	0.42	0/1656	0.72	1/2266 (0.0%)
All	All	0.42	0/13028	0.70	5/17804 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	LEU	CA-CB-CG	8.80	135.54	115.30
1	A	119	LEU	CA-CB-CG	8.34	134.47	115.30
1	E	119	LEU	CA-CB-CG	7.65	132.89	115.30
1	G	119	LEU	CA-CB-CG	7.58	132.74	115.30
2	H	43	GLN	N-CA-C	5.07	124.70	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1567	0	1514	85	0
1	C	1567	0	1514	114	0
1	E	1567	0	1514	123	0
1	G	1567	0	1514	80	0
2	B	1614	0	1551	87	0
2	D	1614	0	1551	113	0
2	F	1614	0	1551	99	0
2	H	1614	0	1551	102	0
3	B	26	0	24	3	0
3	D	26	0	24	3	0
3	F	26	0	24	3	0
3	H	26	0	24	5	0
4	A	7	0	0	1	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	10	0	0	2	0
4	E	6	0	0	1	0
4	F	4	0	0	0	0
4	G	8	0	0	3	0
4	H	10	0	0	1	0
All	All	12882	0	12356	761	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 30.

All (761) 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)
2:F:6:GLN:HB2	2:F:111:GLN:HE22	1.23	1.02
2:D:34:MET:HE3	2:D:79:VAL:HB	1.47	0.96
2:F:124:PRO:HB3	2:F:150:TYR:HB3	1.50	0.94
1:E:68:LEU:HD23	1:E:73:ALA:HB2	1.49	0.94
1:A:24:SER:H	1:A:29:ILE:HD11	1.32	0.93
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.51	0.92
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.50	0.92
2:B:111:GLN:H	2:B:111:GLN:NE2	1.68	0.91
2:D:17:SER:HB2	4:D:361:HOH:O	1.69	0.91
2:D:111:GLN:H	2:D:111:GLN:NE2	1.68	0.91
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.52	0.90
1:G:185:ARG:HA	1:G:185:ARG:NH1	1.87	0.89
1:C:24:SER:H	1:C:29:ILE:HD11	1.36	0.89
1:C:185:ARG:NH1	1:C:185:ARG:HA	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HA	1:A:185:ARG:NH1	1.88	0.88
1:A:87:ILE:HG12	1:A:105:LYS:HG2	1.54	0.87
2:D:111:GLN:H	2:D:111:GLN:HE21	1.18	0.87
2:F:6:GLN:HB2	2:F:111:GLN:NE2	1.90	0.86
1:C:49:LEU:HA	1:C:60:VAL:HG21	1.58	0.85
2:H:52:TYR:HD2	2:H:55:ASP:HB2	1.41	0.85
2:D:38:ARG:HB2	2:D:48:ILE:HD11	1.58	0.85
1:C:91:ALA:HB2	1:C:100:PHE:CD2	2.12	0.85
2:B:35:GLN:HG2	2:B:47:TRP:CH2	2.11	0.84
1:C:37:TRP:CZ3	1:C:90:CYS:HB3	2.12	0.84
1:C:85:GLU:HG3	1:C:107:THR:HA	1.59	0.83
1:E:160:GLY:H	2:H:1:GLU:CD	1.83	0.82
1:E:185:ARG:NH1	1:E:185:ARG:HA	1.94	0.81
1:C:95:SER:O	1:C:96:ASN:HB3	1.80	0.81
2:B:34:MET:HE3	2:B:79:VAL:HB	1.63	0.81
2:F:35:GLN:HG2	2:F:47:TRP:CH2	2.15	0.81
2:H:17:SER:HA	2:H:86:LEU:CD2	2.11	0.81
1:E:65:SER:HB2	1:E:76:THR:HB	1.61	0.80
2:D:40:ARG:HD3	2:D:43:GLN:NE2	1.97	0.80
1:C:39:GLN:HB2	1:C:49:LEU:HD11	1.64	0.80
1:G:36:ASN:HD22	1:G:37:TRP:N	1.79	0.79
1:E:20:LEU:HD23	1:E:104:THR:HG21	1.62	0.79
2:B:40:ARG:O	2:B:42:GLY:N	2.16	0.78
1:A:134:LEU:HB2	1:A:180:LEU:HB3	1.66	0.78
1:C:134:LEU:HB2	1:C:180:LEU:HB3	1.67	0.77
2:H:34:MET:HE3	2:H:79:VAL:HB	1.67	0.77
2:F:6:GLN:CB	2:F:111:GLN:HE22	1.97	0.76
2:D:34:MET:CE	2:D:79:VAL:HB	2.15	0.76
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.66	0.76
2:B:6:GLN:HE21	2:B:110:GLY:HA3	1.49	0.76
1:A:72:LYS:HB2	1:A:72:LYS:NZ	2.01	0.76
1:G:185:ARG:HA	1:G:185:ARG:CZ	2.16	0.75
1:A:17:THR:HA	1:A:77:ILE:O	1.86	0.75
1:G:181:THR:HG23	4:G:213:HOH:O	1.87	0.74
2:F:30:THR:HB	2:F:54:GLY:HA3	1.66	0.74
1:A:63:ARG:NH2	1:A:81:GLN:HG3	2.02	0.74
2:D:35:GLN:HG2	2:D:47:TRP:CH2	2.22	0.74
1:C:23:ARG:CZ	1:C:72:LYS:HD3	2.18	0.73
1:E:134:LEU:HB2	1:E:180:LEU:HB3	1.68	0.73
2:F:87:THR:HG22	2:F:88:SER:N	2.05	0.72
2:H:111:GLN:H	2:H:111:GLN:HE21	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:ILE:HA	2:F:64:PHE:CD2	2.25	0.72
2:D:40:ARG:HG2	2:D:92:ALA:HB2	1.71	0.71
1:E:42:PRO:O	1:E:43:ASP:HB2	1.90	0.71
1:A:48:GLY:HA3	2:B:107:ASP:HA	1.71	0.71
2:D:51:ILE:HB	2:D:70:LEU:HD23	1.70	0.71
1:C:185:ARG:CZ	1:C:185:ARG:HA	2.20	0.71
1:G:134:LEU:HB2	1:G:180:LEU:HB3	1.71	0.70
2:D:26:GLY:O	2:D:27:TYR:HB3	1.92	0.70
1:E:185:ARG:HA	1:E:185:ARG:CZ	2.20	0.70
2:H:40:ARG:HB3	2:H:41:PRO:HD2	1.74	0.70
1:A:185:ARG:HA	1:A:185:ARG:CZ	2.21	0.70
1:E:36:ASN:HD22	1:E:37:TRP:N	1.89	0.70
1:E:20:LEU:H	1:E:20:LEU:HD12	1.57	0.69
1:A:65:SER:OG	1:A:76:THR:HB	1.93	0.69
2:F:51:ILE:HB	2:F:70:LEU:HD23	1.75	0.69
1:E:169:GLN:NE2	1:E:175:MET:HB3	2.08	0.69
1:E:48:GLY:HA3	2:F:107:ASP:HA	1.75	0.69
2:H:60:TYR:HE2	2:H:69:THR:HA	1.58	0.69
1:C:159:GLN:CD	1:C:159:GLN:H	1.96	0.69
1:G:164:THR:HG22	2:H:174:VAL:CG1	2.24	0.68
1:E:95:SER:O	1:E:96:ASN:HB3	1.92	0.68
1:G:38:ILE:HD13	2:H:109:TRP:CZ2	2.28	0.68
2:D:12:ALA:O	2:D:117:VAL:HA	1.94	0.68
1:E:57:ALA:HB3	1:E:60:VAL:CG2	2.24	0.67
1:C:81:GLN:O	1:C:108:VAL:HG21	1.93	0.67
1:A:24:SER:N	1:A:29:ILE:HD11	2.09	0.67
1:C:18:VAL:HG22	1:C:19:THR:H	1.60	0.67
1:C:38:ILE:HB	1:C:89:ILE:HG13	1.77	0.67
2:F:34:MET:HE3	2:F:79:VAL:HB	1.77	0.67
1:E:86:ALA:O	1:E:106:VAL:HB	1.93	0.67
1:E:159:GLN:H	1:E:159:GLN:CD	1.97	0.67
1:C:23:ARG:NH1	1:C:72:LYS:HD3	2.10	0.67
1:C:85:GLU:HG3	1:C:106:VAL:O	1.94	0.67
1:C:169:GLN:NE2	1:C:175:MET:HB3	2.10	0.66
2:B:57:ASP:OD2	2:B:59:ARG:NH1	2.28	0.66
2:B:48:ILE:HA	2:B:64:PHE:CD2	2.30	0.66
2:B:30:THR:HB	2:B:54:GLY:HA3	1.76	0.66
1:G:171:ASN:OD1	1:G:173:LYS:HB2	1.96	0.66
1:C:29:ILE:HD13	1:C:72:LYS:HA	1.77	0.66
1:C:37:TRP:HD1	1:C:50:ILE:HB	1.59	0.66
1:E:20:LEU:HD23	1:E:104:THR:CG2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASN:OD1	1:C:173:LYS:HB2	1.96	0.66
1:E:171:ASN:OD1	1:E:173:LYS:HB2	1.96	0.66
2:F:57:ASP:OD2	2:F:59:ARG:NH1	2.29	0.65
1:G:206:LYS:HD3	2:H:134:ALA:HB1	1.78	0.65
2:D:4:LEU:CD2	2:D:24:THR:HG22	2.25	0.65
2:F:6:GLN:NE2	2:F:112:GLY:HA2	2.11	0.65
2:H:34:MET:CE	2:H:79:VAL:HB	2.26	0.65
1:A:159:GLN:CD	1:A:159:GLN:H	1.99	0.65
1:A:23:ARG:NH2	1:A:72:LYS:HD3	2.11	0.65
2:H:111:GLN:H	2:H:111:GLN:NE2	1.94	0.65
1:G:23:ARG:HH22	1:G:72:LYS:CE	2.08	0.65
2:D:3:GLN:HG3	2:D:25:SER:HB3	1.78	0.65
1:A:164:THR:HG22	2:B:174:VAL:CG1	2.27	0.65
1:E:2:ALA:HB2	1:E:26:SER:HB3	1.79	0.65
2:H:51:ILE:O	2:H:53:PRO:HD3	1.96	0.65
1:G:98:PHE:HB2	2:H:47:TRP:CE3	2.32	0.65
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.27	0.64
1:G:169:GLN:NE2	1:G:175:MET:HB3	2.11	0.64
2:D:48:ILE:HA	2:D:64:PHE:CD2	2.32	0.64
2:D:40:ARG:HB3	2:D:41:PRO:HD2	1.78	0.64
1:G:159:GLN:CD	1:G:159:GLN:H	1.99	0.64
1:G:23:ARG:HH22	1:G:72:LYS:HE2	1.61	0.64
2:F:39:GLN:O	2:F:92:ALA:HB1	1.98	0.64
2:D:198:VAL:O	2:D:215:ILE:HG23	1.97	0.64
2:H:17:SER:HA	2:H:86:LEU:HD23	1.80	0.63
2:H:12:ALA:O	2:H:117:VAL:HA	1.97	0.63
2:D:6:GLN:NE2	2:D:112:GLY:HA2	2.13	0.63
1:E:85:GLU:HG3	1:E:107:THR:HA	1.79	0.63
1:A:82:THR:HA	1:A:108:VAL:HG11	1.80	0.63
1:E:68:LEU:HA	1:E:73:ALA:HA	1.81	0.63
2:H:57:ASP:OD2	2:H:59:ARG:NH1	2.32	0.63
2:F:4:LEU:HD12	2:F:109:TRP:HA	1.80	0.63
1:C:29:ILE:HD12	1:C:29:ILE:N	2.14	0.63
1:A:169:GLN:NE2	1:A:175:MET:HB3	2.13	0.63
2:F:37:VAL:HG13	2:F:46:GLU:O	1.98	0.63
2:D:40:ARG:HD3	2:D:43:GLN:HE22	1.63	0.62
2:D:39:GLN:O	2:D:92:ALA:HB1	1.98	0.62
2:B:17:SER:HA	2:B:86:LEU:HD22	1.79	0.62
2:D:215:ILE:O	2:D:215:ILE:HG13	1.99	0.62
1:E:20:LEU:HD12	1:E:20:LEU:N	2.14	0.62
2:B:62:GLN:OE1	2:F:59:ARG:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:ILE:HD13	2:H:109:TRP:HZ2	1.64	0.62
1:C:37:TRP:CE2	1:C:75:LEU:HB2	2.35	0.61
1:C:7:GLU:OE2	1:C:20:LEU:HA	2.00	0.61
1:A:57:ALA:HB1	1:A:58:PRO:HD2	1.82	0.61
1:A:206:LYS:HD3	2:B:134:ALA:HB1	1.80	0.61
1:C:164:THR:HG22	2:D:174:VAL:CG1	2.30	0.61
1:A:63:ARG:CZ	1:A:81:GLN:HG3	2.31	0.61
1:G:35:ALA:HB3	1:G:53:THR:HA	1.80	0.61
2:B:4:LEU:HG	2:B:24:THR:HG22	1.83	0.61
2:B:35:GLN:HG2	2:B:47:TRP:HH2	1.62	0.61
2:D:6:GLN:OE1	2:D:113:THR:HG23	2.01	0.61
1:G:96:ASN:O	1:G:97:GLN:HB3	2.01	0.61
2:D:70:LEU:HD12	2:D:70:LEU:N	2.16	0.60
1:A:18:VAL:HG12	1:A:77:ILE:HB	1.82	0.60
2:F:198:VAL:O	2:F:215:ILE:HG23	2.02	0.60
1:A:72:LYS:HB2	1:A:72:LYS:HZ3	1.63	0.60
1:A:85:GLU:HG3	1:A:107:THR:HA	1.84	0.60
1:E:53:THR:CG2	1:E:68:LEU:HG	2.32	0.60
1:E:7:GLU:O	1:E:104:THR:HG23	2.01	0.60
1:C:24:SER:N	1:C:29:ILE:HD11	2.14	0.60
2:H:31:THR:HA	2:H:52:TYR:OH	2.01	0.60
1:A:42:PRO:O	1:A:43:ASP:HB2	2.01	0.60
2:D:59:ARG:HG2	2:D:59:ARG:HH11	1.67	0.60
1:C:65:SER:O	1:C:75:LEU:HD12	2.01	0.60
1:G:164:THR:HG22	2:H:174:VAL:HG12	1.83	0.59
1:E:96:ASN:HA	3:F:353:ECO:C3	2.33	0.59
2:H:6:GLN:HG2	2:H:22:CYS:SG	2.42	0.59
2:B:24:THR:HG1	2:B:29:PHE:HD1	1.48	0.59
1:A:50:ILE:HD13	1:A:56:ARG:HA	1.83	0.59
1:A:8:SER:HB3	2:D:166:SER:OG	2.02	0.59
2:H:127:TYR:HE2	2:H:148:LYS:HE2	1.65	0.59
2:D:6:GLN:HB3	2:D:113:THR:CG2	2.32	0.59
1:G:94:PHE:O	1:G:95:SER:O	2.21	0.59
2:B:215:ILE:O	2:B:215:ILE:HG13	2.02	0.59
2:F:16:ALA:O	2:F:86:LEU:HD23	2.02	0.59
2:H:17:SER:HA	2:H:86:LEU:HD21	1.84	0.59
1:C:209:SER:O	1:C:211:ALA:N	2.36	0.59
2:F:23:ARG:HG2	2:F:78:ILE:HG12	1.85	0.59
1:A:164:THR:HG22	2:B:174:VAL:HG12	1.82	0.59
2:B:152:PRO:O	2:B:204:HIS:HE1	1.86	0.59
1:E:57:ALA:HB3	1:E:60:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:PRO:O	1:C:43:ASP:HB2	2.01	0.59
2:H:171:PHE:HB3	2:H:172:PRO:HD2	1.84	0.59
2:B:46:GLU:OE1	2:B:63:LYS:HE2	2.02	0.59
1:C:18:VAL:HG22	1:C:19:THR:N	2.17	0.59
2:D:29:PHE:CD2	2:D:77:SER:HA	2.38	0.59
2:B:23:ARG:HB3	2:B:78:ILE:HG12	1.84	0.59
1:E:17:THR:HG23	1:E:78:THR:HA	1.85	0.59
2:B:111:GLN:N	2:B:111:GLN:NE2	2.47	0.58
2:F:10:GLU:HG2	2:F:18:VAL:CG1	2.33	0.58
2:F:51:ILE:CG2	2:F:70:LEU:HD23	2.34	0.58
2:H:198:VAL:O	2:H:215:ILE:HG23	2.04	0.58
2:B:43:GLN:O	2:B:44:GLY:O	2.20	0.58
2:B:40:ARG:HB3	2:B:41:PRO:HD2	1.85	0.58
2:B:54:GLY:O	2:B:55:ASP:HB2	2.04	0.58
2:F:182:LEU:HD23	2:F:182:LEU:C	2.24	0.58
1:C:85:GLU:CG	1:C:107:THR:HA	2.33	0.58
2:B:31:THR:HA	2:B:52:TYR:OH	2.03	0.58
2:F:19:LYS:HE2	2:F:80:TYR:CD2	2.38	0.58
1:C:17:THR:HA	1:C:77:ILE:O	2.03	0.58
2:D:2:VAL:HB	2:D:108:TYR:CE1	2.39	0.58
2:D:6:GLN:HE22	2:D:112:GLY:HA2	1.68	0.58
2:D:2:VAL:HB	2:D:108:TYR:CD1	2.37	0.58
1:A:171:ASN:OD1	1:A:173:LYS:HB2	2.04	0.58
1:E:36:ASN:HD22	1:E:37:TRP:H	1.51	0.57
2:F:152:PRO:O	2:F:204:HIS:HE1	1.87	0.57
1:C:34:TYR:HB3	1:C:52:GLY:HA2	1.85	0.57
2:F:124:PRO:CB	2:F:150:TYR:HB3	2.31	0.57
1:E:53:THR:HG21	1:E:68:LEU:HG	1.86	0.57
1:G:82:THR:HA	1:G:108:VAL:HG11	1.85	0.57
1:G:20:LEU:N	1:G:20:LEU:HD12	2.19	0.57
2:B:182:LEU:HD23	2:B:182:LEU:C	2.24	0.57
2:B:198:VAL:O	2:B:215:ILE:HG23	2.03	0.57
2:B:127:TYR:HE2	2:B:148:LYS:HE2	1.68	0.57
1:E:18:VAL:HG22	1:E:19:THR:N	2.20	0.57
3:D:352:ECO:H192	3:D:352:ECO:C7	2.34	0.57
1:A:56:ARG:NE	1:A:62:ALA:HA	2.20	0.57
2:H:182:LEU:C	2:H:182:LEU:HD23	2.25	0.57
1:G:36:ASN:C	1:G:36:ASN:HD22	2.05	0.57
2:F:87:THR:CG2	2:F:88:SER:N	2.68	0.57
2:D:18:VAL:HG22	2:D:86:LEU:HD21	1.86	0.57
1:A:29:ILE:N	1:A:29:ILE:HD12	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG12	2:B:38:ARG:N	2.20	0.56
1:G:42:PRO:O	1:G:43:ASP:HB2	2.05	0.56
1:G:56:ARG:HD3	1:G:60:VAL:O	2.05	0.56
1:C:83:GLU:C	1:C:85:GLU:H	2.09	0.56
2:F:127:TYR:HE2	2:F:148:LYS:HE2	1.68	0.56
2:D:1:GLU:O	2:D:26:GLY:HA3	2.06	0.56
2:D:64:PHE:HB3	2:D:68:ALA:HB3	1.87	0.56
1:A:24:SER:HB3	1:A:29:ILE:HD11	1.88	0.56
2:F:171:PHE:HB3	2:F:172:PRO:HD2	1.86	0.56
1:E:37:TRP:CE2	1:E:75:LEU:HB2	2.40	0.56
1:G:146:VAL:HG12	1:G:199:HIS:HB2	1.88	0.55
2:H:124:PRO:CB	2:H:150:TYR:HB3	2.33	0.55
2:D:48:ILE:HG12	2:D:64:PHE:CE2	2.41	0.55
1:C:187:TRP:CZ2	1:C:210:ALA:HA	2.41	0.55
2:H:60:TYR:CE2	2:H:69:THR:HA	2.41	0.55
1:E:88:TYR:CE2	1:E:106:VAL:HG21	2.42	0.55
2:H:175:LEU:HD13	2:H:180:TYR:CE1	2.41	0.55
1:E:81:GLN:O	1:E:108:VAL:HG11	2.07	0.55
1:G:15:GLY:O	1:G:79:GLY:HA2	2.07	0.55
2:F:40:ARG:O	2:F:41:PRO:C	2.45	0.55
1:E:14:PRO:HA	1:E:80:ALA:O	2.06	0.55
1:E:152:VAL:HG22	1:E:193:TYR:CD2	2.42	0.55
1:A:152:VAL:HG22	1:A:193:TYR:CD2	2.42	0.55
1:E:11:THR:HG22	1:E:107:THR:HB	1.87	0.55
2:H:143:LEU:H	2:H:143:LEU:HD22	1.72	0.55
1:E:31:THR:O	1:E:31:THR:HG22	2.07	0.55
1:E:20:LEU:O	1:E:74:ALA:HB1	2.07	0.54
1:G:56:ARG:HB2	1:G:56:ARG:NH1	2.22	0.54
1:G:152:VAL:HG12	1:G:190:HIS:CD2	2.42	0.54
2:D:51:ILE:HB	2:D:70:LEU:CD2	2.37	0.54
2:D:83:LEU:HD11	2:D:94:TYR:CE2	2.43	0.54
2:H:152:PRO:O	2:H:204:HIS:HE1	1.90	0.54
2:D:182:LEU:HD23	2:D:182:LEU:C	2.27	0.54
1:E:38:ILE:N	1:E:38:ILE:HD12	2.22	0.54
1:E:68:LEU:HD23	1:E:73:ALA:CB	2.32	0.54
1:C:95:SER:O	1:C:96:ASN:CB	2.52	0.54
2:B:150:TYR:CE1	2:B:155:VAL:HG13	2.42	0.54
2:B:111:GLN:H	2:B:111:GLN:HE21	1.51	0.54
2:F:38:ARG:HB3	2:F:48:ILE:HD11	1.90	0.54
1:G:50:ILE:HD13	1:G:56:ARG:HA	1.88	0.54
1:C:72:LYS:HB2	1:C:72:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:215:ILE:HG13	2:F:215:ILE:O	2.07	0.54
2:D:39:GLN:C	2:D:92:ALA:HB1	2.29	0.54
2:F:87:THR:HG22	2:F:88:SER:H	1.73	0.54
2:F:40:ARG:HA	2:F:92:ALA:HB2	1.88	0.54
1:C:152:VAL:HG22	1:C:193:TYR:CD2	2.43	0.54
2:H:70:LEU:HD11	2:H:81:LEU:HD23	1.90	0.54
1:E:164:THR:CB	2:F:172:PRO:HG2	2.38	0.53
2:D:13:ARG:HD2	2:D:13:ARG:N	2.23	0.53
2:D:152:PRO:O	2:D:204:HIS:HE1	1.91	0.53
2:D:127:TYR:HE2	2:D:148:LYS:HE2	1.72	0.53
1:A:9:ALA:O	1:A:10:LEU:HD23	2.07	0.53
1:A:63:ARG:HD3	1:A:79:GLY:O	2.07	0.53
1:E:50:ILE:HD13	1:E:56:ARG:HA	1.90	0.53
2:F:52:TYR:CD2	2:F:55:ASP:HB2	2.44	0.53
1:E:57:ALA:HB3	1:E:60:VAL:HG23	1.89	0.53
2:H:35:GLN:HG2	2:H:47:TRP:CH2	2.43	0.53
2:D:17:SER:HA	2:D:86:LEU:CD2	2.38	0.53
2:H:11:LEU:HD22	2:H:116:THR:HB	1.91	0.53
1:C:40:GLU:HB3	1:C:87:ILE:HB	1.91	0.53
1:G:30:THR:HG23	1:G:33:HIS:CE1	2.43	0.53
2:B:176:GLN:OE1	2:B:181:THR:HG21	2.09	0.53
1:E:29:ILE:N	1:E:29:ILE:HD12	2.23	0.53
2:H:6:GLN:NE2	2:H:112:GLY:H	2.07	0.53
1:E:37:TRP:CZ3	1:E:90:CYS:HB3	2.44	0.53
2:F:51:ILE:CB	2:F:70:LEU:HD23	2.38	0.53
2:D:29:PHE:CE2	2:D:77:SER:HA	2.44	0.53
1:E:82:THR:HA	1:E:108:VAL:HG11	1.91	0.53
2:F:52:TYR:HD2	2:F:55:ASP:HB2	1.73	0.53
2:D:67:LYS:HG3	2:D:68:ALA:H	1.73	0.53
2:F:86:LEU:HB3	2:F:117:VAL:HG21	1.91	0.53
2:F:36:TRP:CE3	2:F:81:LEU:HD12	2.44	0.53
1:E:52:GLY:O	1:E:53:THR:HB	2.09	0.52
2:D:35:GLN:HG2	2:D:47:TRP:HH2	1.69	0.52
2:D:176:GLN:OE1	2:D:181:THR:HG21	2.09	0.52
1:A:151:LYS:HB2	1:A:194:SER:HB3	1.91	0.52
1:E:39:GLN:O	1:E:46:PHE:HA	2.08	0.52
2:B:175:LEU:HD13	2:B:180:TYR:CE1	2.44	0.52
1:C:56:ARG:NH2	1:C:64:PHE:O	2.43	0.52
3:H:354:ECO:H192	3:H:354:ECO:C7	2.40	0.52
2:F:176:GLN:O	2:F:177:SER:HB2	2.09	0.52
1:A:38:ILE:HD13	2:B:109:TRP:CZ2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:THR:HA	1:C:108:VAL:HB	1.91	0.52
2:F:6:GLN:NE2	2:F:112:GLY:N	2.58	0.52
2:D:34:MET:HB3	2:D:51:ILE:HG22	1.92	0.52
2:D:111:GLN:N	2:D:111:GLN:NE2	2.50	0.52
2:H:176:GLN:O	2:H:177:SER:HB2	2.09	0.52
2:B:1:GLU:CD	2:B:1:GLU:O	2.48	0.52
1:C:119:LEU:HD21	1:C:195:CYS:HB3	1.91	0.52
2:F:6:GLN:HE22	2:F:112:GLY:HA2	1.75	0.52
2:H:150:TYR:CE1	2:H:155:VAL:HG13	2.45	0.52
2:H:57:ASP:OD1	2:H:59:ARG:HD2	2.09	0.52
1:G:34:TYR:HE2	2:H:103:TYR:CE1	2.27	0.52
2:F:40:ARG:HA	2:F:92:ALA:CB	2.40	0.52
1:E:91:ALA:HB2	1:E:100:PHE:CE2	2.44	0.52
1:C:97:GLN:HG3	1:C:97:GLN:O	2.10	0.52
2:D:28:SER:OG	2:D:31:THR:OG1	2.23	0.52
2:F:6:GLN:NE2	2:F:112:GLY:CA	2.73	0.52
1:C:37:TRP:CD1	1:C:50:ILE:HB	2.43	0.52
1:G:116:SER:HA	4:G:215:HOH:O	2.09	0.52
1:E:24:SER:H	1:E:29:ILE:HD11	1.74	0.52
1:A:85:GLU:HG3	1:A:106:VAL:O	2.10	0.52
1:A:7:GLU:O	1:A:104:THR:HA	2.10	0.52
1:E:2:ALA:HB3	1:E:94:PHE:CE1	2.44	0.51
2:D:36:TRP:CE3	2:D:81:LEU:HD12	2.45	0.51
2:D:16:ALA:O	2:D:86:LEU:HD22	2.10	0.51
1:A:38:ILE:HD13	2:B:109:TRP:HZ2	1.74	0.51
1:C:161:MET:HA	1:C:179:TYR:O	2.10	0.51
2:B:143:LEU:H	2:B:143:LEU:HD22	1.75	0.51
2:F:175:LEU:HD13	2:F:180:TYR:CE1	2.45	0.51
1:E:4:VAL:HG22	1:E:92:LEU:HD12	1.92	0.51
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.46	0.51
1:G:152:VAL:HG22	1:G:193:TYR:CD2	2.46	0.51
1:E:30:THR:C	1:E:32:SER:H	2.13	0.51
1:A:98:PHE:HB2	2:B:47:TRP:CE3	2.46	0.51
2:H:87:THR:O	2:H:88:SER:C	2.49	0.51
1:E:36:ASN:HA	1:E:50:ILE:O	2.10	0.51
2:F:176:GLN:OE1	2:F:181:THR:HG21	2.10	0.51
1:C:56:ARG:HH21	1:C:62:ALA:CA	2.24	0.51
2:B:124:PRO:CB	2:B:150:TYR:HB3	2.33	0.51
1:C:98:PHE:HB2	2:D:47:TRP:CE3	2.45	0.51
1:E:202:HIS:HE1	4:E:213:HOH:O	1.92	0.51
3:B:351:ECO:C7	3:B:351:ECO:H192	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:THR:HG22	2:D:174:VAL:HG12	1.93	0.51
1:G:57:ALA:HB3	1:G:60:VAL:CG2	2.40	0.51
2:B:67:LYS:HE3	2:B:90:ASP:OD2	2.10	0.51
1:E:151:LYS:HB2	1:E:194:SER:HB3	1.92	0.51
1:G:57:ALA:HB3	1:G:60:VAL:HG21	1.93	0.51
1:C:152:VAL:HG13	1:C:193:TYR:CE2	2.46	0.51
2:D:111:GLN:N	2:D:111:GLN:HE21	1.96	0.51
1:C:57:ALA:HB3	1:C:60:VAL:HG23	1.92	0.51
2:H:6:GLN:HA	2:H:21:SER:O	2.10	0.51
2:D:67:LYS:HG3	2:D:68:ALA:N	2.26	0.51
1:G:100:PHE:CG	2:H:45:LEU:HB2	2.46	0.51
1:C:53:THR:CG2	1:C:68:LEU:HG	2.40	0.51
1:G:23:ARG:HH11	1:G:23:ARG:HB2	1.76	0.50
1:C:56:ARG:HH21	1:C:62:ALA:HA	1.76	0.50
1:C:23:ARG:HH11	1:C:23:ARG:HB2	1.76	0.50
2:D:171:PHE:HB3	2:D:172:PRO:HD2	1.92	0.50
1:E:164:THR:HB	2:F:172:PRO:HG2	1.93	0.50
1:E:82:THR:HA	1:E:108:VAL:CG1	2.41	0.50
2:H:40:ARG:HA	2:H:92:ALA:HB2	1.92	0.50
2:D:70:LEU:N	2:D:70:LEU:CD1	2.74	0.50
2:H:176:GLN:OE1	2:H:181:THR:HG21	2.11	0.50
1:E:152:VAL:HG13	1:E:193:TYR:CE2	2.47	0.50
1:A:29:ILE:HD13	1:A:71:ASP:O	2.10	0.50
1:E:19:THR:HG23	1:E:75:LEU:O	2.11	0.50
1:C:152:VAL:HG22	1:C:193:TYR:HD2	1.77	0.50
1:E:9:ALA:O	1:E:10:LEU:HD23	2.12	0.50
1:E:94:PHE:O	1:E:95:SER:O	2.30	0.50
1:C:81:GLN:O	1:C:108:VAL:HG11	2.12	0.50
2:F:40:ARG:HB3	2:F:41:PRO:HD2	1.94	0.50
1:E:152:VAL:HG12	1:E:190:HIS:CD2	2.47	0.50
1:G:30:THR:OG1	1:G:31:THR:N	2.44	0.50
1:A:161:MET:HA	1:A:179:TYR:O	2.11	0.50
2:F:122:THR:HG21	2:F:179:LEU:HD21	1.94	0.50
2:H:6:GLN:HE21	2:H:110:GLY:HA3	1.76	0.50
2:F:87:THR:CG2	2:F:88:SER:H	2.25	0.50
2:F:152:PRO:HD2	2:F:206:ALA:CB	2.42	0.50
1:E:91:ALA:HB2	1:E:100:PHE:CD2	2.47	0.50
1:A:24:SER:CB	1:A:29:ILE:HD11	2.42	0.50
2:B:176:GLN:O	2:B:177:SER:HB2	2.11	0.50
1:E:28:ALA:C	1:E:29:ILE:HD12	2.32	0.49
2:B:52:TYR:HD2	2:B:55:ASP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HB2	1:A:78:THR:O	2.11	0.49
1:E:164:THR:HG22	2:F:174:VAL:CG1	2.42	0.49
2:F:36:TRP:CD2	2:F:81:LEU:HD12	2.47	0.49
2:H:81:LEU:HD13	2:H:81:LEU:C	2.32	0.49
2:F:6:GLN:NE2	2:F:112:GLY:H	2.10	0.49
2:B:152:PRO:HD2	2:B:206:ALA:CB	2.43	0.49
1:C:23:ARG:NH2	1:C:72:LYS:HD3	2.26	0.49
2:H:215:ILE:HG13	2:H:215:ILE:O	2.11	0.49
2:B:97:SER:HB3	2:B:109:TRP:CD2	2.47	0.49
1:C:146:VAL:HG12	1:C:199:HIS:HB2	1.95	0.49
1:A:87:ILE:HG12	1:A:105:LYS:CG	2.37	0.49
1:E:98:PHE:HD1	2:F:47:TRP:CZ3	2.31	0.49
1:G:17:THR:HG23	1:G:78:THR:HA	1.92	0.49
1:E:189:ARG:O	1:E:189:ARG:HG2	2.13	0.49
2:F:122:THR:HG23	2:F:151:PHE:HB3	1.94	0.49
1:G:189:ARG:HG2	1:G:189:ARG:O	2.13	0.49
1:E:29:ILE:HG22	1:E:68:LEU:HD21	1.95	0.49
2:D:176:GLN:O	2:D:177:SER:HB2	2.12	0.49
2:H:67:LYS:HG3	2:H:68:ALA:H	1.78	0.49
1:C:206:LYS:HD3	2:D:134:ALA:HB1	1.93	0.49
2:F:4:LEU:CD1	2:F:97:SER:HA	2.42	0.49
2:H:37:VAL:HG11	2:H:45:LEU:HB3	1.94	0.49
2:F:178:ASP:OD1	2:H:28:SER:HB2	2.13	0.49
2:H:40:ARG:O	2:H:41:PRO:C	2.51	0.49
2:B:17:SER:HB3	2:B:84:ASN:HA	1.95	0.49
2:B:99:GLY:HA3	2:B:105:THR:HG1	1.77	0.49
1:E:119:LEU:HD21	1:E:195:CYS:HB3	1.94	0.49
1:C:49:LEU:HA	1:C:60:VAL:CG2	2.37	0.48
2:H:70:LEU:N	2:H:70:LEU:HD12	2.28	0.48
1:A:7:GLU:O	1:A:104:THR:HG23	2.13	0.48
2:B:171:PHE:HB3	2:B:172:PRO:HD2	1.94	0.48
1:E:4:VAL:HG11	1:E:22:CYS:SG	2.53	0.48
2:B:36:TRP:CD1	2:B:70:LEU:HD11	2.49	0.48
2:D:1:GLU:HA	2:D:1:GLU:OE1	2.13	0.48
1:G:96:ASN:HA	3:H:354:ECO:C3	2.44	0.48
2:F:60:TYR:CE2	2:F:69:THR:HA	2.48	0.48
1:A:129:THR:O	1:A:129:THR:HG22	2.13	0.48
1:A:112:LYS:C	1:A:112:LYS:HD3	2.34	0.48
1:E:146:VAL:HG12	1:E:199:HIS:HB2	1.96	0.48
2:D:34:MET:HE2	2:D:79:VAL:CG2	2.43	0.48
2:H:52:TYR:CD2	2:H:55:ASP:HB2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLU:OE1	1:E:7:GLU:N	2.46	0.48
2:H:22:CYS:HB3	2:H:34:MET:CE	2.43	0.48
2:H:60:TYR:N	2:H:60:TYR:CD1	2.81	0.48
2:H:152:PRO:HD2	2:H:206:ALA:CB	2.43	0.48
2:B:111:GLN:N	2:B:111:GLN:HE21	2.10	0.48
1:E:19:THR:HA	1:E:75:LEU:O	2.13	0.48
1:E:18:VAL:HG12	1:E:77:ILE:HB	1.94	0.48
1:C:137:THR:HB	2:D:171:PHE:CZ	2.48	0.48
1:G:96:ASN:HA	3:H:354:ECO:C2	2.43	0.48
1:C:93:TRP:CE3	1:C:93:TRP:HA	2.48	0.48
2:H:27:TYR:HD2	2:H:32:TYR:CD2	2.32	0.48
1:A:85:GLU:OE1	1:A:107:THR:HG23	2.13	0.48
1:G:17:THR:HG23	1:G:77:ILE:O	2.14	0.48
2:F:35:GLN:HG2	2:F:47:TRP:HH2	1.75	0.48
2:D:64:PHE:C	2:D:66:GLY:N	2.66	0.48
2:F:78:ILE:HG22	2:F:79:VAL:N	2.29	0.48
1:E:81:GLN:HB3	1:E:83:GLU:HG2	1.96	0.48
1:C:12:THR:O	1:C:108:VAL:HA	2.14	0.48
2:D:17:SER:HA	2:D:86:LEU:HD22	1.94	0.47
2:D:64:PHE:O	2:D:66:GLY:N	2.47	0.47
2:D:40:ARG:O	2:D:41:PRO:C	2.52	0.47
2:B:24:THR:HG21	2:B:27:TYR:OH	2.14	0.47
2:F:48:ILE:HG23	2:F:64:PHE:CG	2.49	0.47
2:D:52:TYR:HD2	2:D:55:ASP:HB2	1.79	0.47
1:E:24:SER:HB2	1:E:92:LEU:CD1	2.44	0.47
2:D:124:PRO:CB	2:D:150:TYR:HB3	2.33	0.47
1:C:29:ILE:HD12	1:C:29:ILE:H	1.78	0.47
1:C:91:ALA:HA	1:C:99:ILE:O	2.13	0.47
2:H:48:ILE:HA	2:H:64:PHE:CD2	2.49	0.47
1:C:152:VAL:HG12	1:C:190:HIS:CD2	2.49	0.47
1:G:151:LYS:HB2	1:G:194:SER:HB3	1.95	0.47
1:C:39:GLN:CB	1:C:49:LEU:HD11	2.39	0.47
2:H:29:PHE:CE2	2:H:53:PRO:HB3	2.49	0.47
1:G:152:VAL:CG2	1:G:157:VAL:HG11	2.44	0.47
2:F:60:TYR:HE2	2:F:68:ALA:O	1.97	0.47
1:E:34:TYR:O	1:E:35:ALA:C	2.52	0.47
2:F:150:TYR:CE1	2:F:155:VAL:HG13	2.49	0.47
1:A:189:ARG:O	1:A:189:ARG:HG2	2.15	0.47
2:H:122:THR:HG21	2:H:179:LEU:HD21	1.96	0.47
2:F:34:MET:HG2	2:F:79:VAL:HG21	1.96	0.47
2:F:4:LEU:HB2	2:F:109:TRP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:VAL:CG2	2:F:181:THR:HG23	2.44	0.47
2:D:26:GLY:O	2:D:27:TYR:CB	2.62	0.47
2:B:34:MET:CE	2:B:79:VAL:HB	2.40	0.47
1:G:134:LEU:HD11	1:G:187:TRP:CZ3	2.50	0.47
2:H:39:GLN:O	2:H:92:ALA:HB1	2.14	0.47
2:F:51:ILE:HB	2:F:70:LEU:CD2	2.43	0.47
2:H:83:LEU:HD11	2:H:94:TYR:CE2	2.50	0.47
1:G:38:ILE:CD1	2:H:109:TRP:HZ2	2.27	0.47
4:A:217:HOH:O	2:B:44:GLY:HA2	2.15	0.47
1:G:152:VAL:CG1	1:G:190:HIS:CD2	2.98	0.47
2:D:152:PRO:HD2	2:D:206:ALA:CB	2.45	0.47
2:F:40:ARG:HD3	2:F:43:GLN:NE2	2.30	0.47
1:E:137:THR:HB	2:F:171:PHE:CZ	2.50	0.47
1:A:119:LEU:HD21	1:A:195:CYS:HB3	1.95	0.47
1:C:209:SER:C	1:C:211:ALA:N	2.68	0.47
2:H:6:GLN:OE1	2:H:113:THR:HG22	2.14	0.47
1:A:95:SER:O	1:A:96:ASN:CB	2.63	0.47
2:B:51:ILE:HB	2:B:70:LEU:HD23	1.97	0.46
1:C:194:SER:HB2	1:C:207:SER:OG	2.14	0.46
2:F:7:SER:O	2:F:113:THR:HG22	2.15	0.46
2:F:4:LEU:HD12	2:F:109:TRP:CA	2.46	0.46
1:A:152:VAL:CG2	1:A:157:VAL:HG11	2.45	0.46
2:F:67:LYS:NZ	2:F:84:ASN:O	2.48	0.46
1:E:112:LYS:HD3	1:E:112:LYS:C	2.35	0.46
1:E:206:LYS:HD3	2:F:134:ALA:HB1	1.97	0.46
2:H:34:MET:O	2:H:50:ALA:HA	2.16	0.46
2:H:122:THR:HG23	2:H:151:PHE:HB3	1.98	0.46
2:B:122:THR:HG23	2:B:151:PHE:HB3	1.97	0.46
1:G:13:SER:O	1:G:14:PRO:C	2.53	0.46
2:D:34:MET:O	2:D:50:ALA:HA	2.16	0.46
1:C:57:ALA:HB1	1:C:58:PRO:HD2	1.96	0.46
2:D:143:LEU:HD22	2:D:143:LEU:H	1.80	0.46
1:A:52:GLY:CA	2:B:103:TYR:HA	2.46	0.46
1:E:68:LEU:CD2	1:E:73:ALA:HB2	2.34	0.46
1:C:152:VAL:CG2	1:C:157:VAL:HG11	2.45	0.46
1:E:12:THR:OG1	1:E:13:SER:N	2.48	0.46
2:D:61:THR:O	2:D:62:GLN:C	2.52	0.46
1:G:20:LEU:O	1:G:74:ALA:HB1	2.15	0.46
2:F:68:ALA:O	2:F:69:THR:HG23	2.16	0.46
2:H:126:VAL:O	2:H:213:LYS:HE3	2.16	0.46
1:G:23:ARG:HH12	1:G:72:LYS:HE3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:LEU:HD23	1:C:104:THR:HB	1.98	0.46
2:F:53:PRO:O	2:F:55:ASP:N	2.42	0.46
1:A:145:VAL:HG13	1:A:145:VAL:O	2.16	0.46
2:D:194:PRO:O	2:D:195:SER:C	2.54	0.46
2:B:37:VAL:CG1	2:B:38:ARG:N	2.80	0.45
2:H:67:LYS:NZ	2:H:84:ASN:O	2.49	0.45
1:C:93:TRP:CD1	2:D:102:LEU:HD13	2.50	0.45
2:D:175:LEU:HD13	2:D:180:TYR:CE1	2.51	0.45
2:H:70:LEU:N	2:H:70:LEU:CD1	2.79	0.45
1:C:30:THR:HA	1:C:68:LEU:HD13	1.98	0.45
1:G:119:LEU:HD21	1:G:195:CYS:HB3	1.96	0.45
1:A:152:VAL:HG13	1:A:193:TYR:CE2	2.52	0.45
1:C:56:ARG:NH2	1:C:62:ALA:O	2.48	0.45
2:F:60:TYR:CD1	2:F:60:TYR:N	2.83	0.45
2:D:40:ARG:HB3	2:D:41:PRO:CD	2.43	0.45
2:B:40:ARG:C	2:B:42:GLY:H	2.19	0.45
1:C:33:HIS:O	1:C:34:TYR:C	2.55	0.45
1:E:14:PRO:HG3	1:E:108:VAL:HG12	1.98	0.45
1:G:56:ARG:HE	1:G:62:ALA:HA	1.82	0.45
1:E:193:TYR:O	1:E:207:SER:HA	2.16	0.45
1:G:112:LYS:HD3	1:G:112:LYS:C	2.36	0.45
1:A:23:ARG:HB2	1:A:23:ARG:HH11	1.82	0.45
1:A:15:GLY:O	1:A:79:GLY:HA2	2.16	0.45
1:E:36:ASN:ND2	1:E:50:ILE:O	2.50	0.45
2:D:122:THR:HG23	2:D:151:PHE:HB3	1.98	0.45
1:C:193:TYR:O	1:C:207:SER:HA	2.17	0.45
2:D:204:HIS:HD2	2:D:207:SER:OG	1.99	0.45
1:G:63:ARG:CZ	1:G:81:GLN:HG2	2.46	0.45
1:E:129:THR:O	1:E:129:THR:HG22	2.17	0.45
2:F:164:LEU:HD23	2:F:186:VAL:HG21	1.97	0.45
2:H:29:PHE:CD1	2:H:77:SER:HA	2.51	0.45
2:H:29:PHE:CZ	2:H:79:VAL:HG23	2.52	0.45
2:B:55:ASP:O	2:B:57:ASP:N	2.50	0.45
1:E:152:VAL:CG1	1:E:190:HIS:CD2	2.99	0.45
1:C:53:THR:HG21	1:C:68:LEU:HG	1.97	0.45
2:D:60:TYR:CE2	2:D:70:LEU:HD13	2.52	0.45
2:D:40:ARG:CG	2:D:92:ALA:HB2	2.43	0.45
2:H:64:PHE:O	2:H:65:LYS:C	2.54	0.45
1:C:129:THR:HG22	1:C:129:THR:O	2.17	0.45
2:F:111:GLN:NE2	2:F:112:GLY:H	2.13	0.45
1:C:37:TRP:HB2	1:C:50:ILE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLN:HB3	2:F:113:THR:CG2	2.46	0.44
1:G:152:VAL:HG13	1:G:193:TYR:CE2	2.52	0.44
1:G:161:MET:HA	1:G:179:TYR:O	2.17	0.44
1:G:9:ALA:O	1:G:10:LEU:HD23	2.17	0.44
2:H:194:PRO:O	2:H:195:SER:C	2.55	0.44
1:E:6:GLN:HG2	1:E:21:THR:O	2.17	0.44
2:B:83:LEU:HD11	2:B:94:TYR:CE2	2.53	0.44
2:F:18:VAL:HG23	2:F:86:LEU:HD21	1.99	0.44
2:F:204:HIS:HD2	2:F:207:SER:OG	2.01	0.44
1:G:56:ARG:NE	1:G:62:ALA:HA	2.31	0.44
1:E:29:ILE:HG23	1:E:33:HIS:CG	2.53	0.44
2:B:34:MET:O	2:B:50:ALA:HA	2.17	0.44
1:E:152:VAL:HG22	1:E:193:TYR:HD2	1.82	0.44
1:A:5:THR:HG22	1:A:6:GLN:N	2.33	0.44
2:B:194:PRO:O	2:B:195:SER:C	2.56	0.44
1:G:129:THR:HG22	1:G:129:THR:O	2.17	0.44
1:C:112:LYS:HD3	1:C:112:LYS:C	2.38	0.44
2:D:55:ASP:OD1	2:H:65:LYS:HE3	2.18	0.44
1:E:2:ALA:HB3	1:E:94:PHE:HE1	1.82	0.44
1:E:96:ASN:OD1	1:E:97:GLN:HG2	2.16	0.44
1:G:56:ARG:CB	1:G:56:ARG:NH1	2.79	0.44
2:F:32:TYR:O	2:F:53:PRO:HD2	2.18	0.44
1:C:66:GLY:HA2	1:C:74:ALA:O	2.17	0.44
1:A:44:HIS:NE2	2:B:93:VAL:HG21	2.33	0.44
1:A:29:ILE:HG21	1:A:73:ALA:HB2	2.00	0.44
2:H:40:ARG:HA	2:H:92:ALA:CB	2.48	0.44
2:H:102:LEU:HD23	3:H:354:ECO:H181	2.00	0.44
2:D:27:TYR:C	2:D:27:TYR:HD2	2.21	0.44
2:D:59:ARG:NH1	2:D:59:ARG:HG2	2.30	0.44
1:G:49:LEU:HD21	1:G:88:TYR:HE1	1.81	0.44
2:B:126:VAL:O	2:B:213:LYS:HE3	2.17	0.44
1:E:152:VAL:CG2	1:E:157:VAL:HG11	2.48	0.44
1:C:179:TYR:OH	2:D:183:SER:HB2	2.18	0.44
2:H:5:GLN:O	2:H:23:ARG:HG2	2.18	0.44
1:C:61:PRO:HB3	1:C:63:ARG:NH1	2.33	0.44
2:D:27:TYR:C	2:D:27:TYR:CD2	2.91	0.44
2:F:40:ARG:HD3	2:F:43:GLN:HE22	1.83	0.44
2:B:17:SER:HB2	2:B:83:LEU:O	2.18	0.44
2:H:33:TRP:CD1	3:H:354:ECO:H161	2.53	0.44
2:H:3:GLN:C	2:H:4:LEU:HD23	2.38	0.44
2:B:12:ALA:O	2:B:117:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:VAL:O	1:G:145:VAL:HG13	2.18	0.44
1:E:208:LEU:HD12	1:E:208:LEU:O	2.17	0.44
1:A:24:SER:HB3	1:A:29:ILE:CD1	2.48	0.44
1:G:25:SER:O	1:G:26:SER:C	2.56	0.44
1:A:57:ALA:O	1:A:60:VAL:HG23	2.18	0.43
2:H:143:LEU:N	2:H:143:LEU:HD22	2.33	0.43
1:A:96:ASN:HB2	3:B:351:ECO:O3	2.18	0.43
1:C:145:VAL:HG13	1:C:145:VAL:O	2.18	0.43
2:H:29:PHE:CG	2:H:77:SER:HA	2.53	0.43
1:A:63:ARG:NE	1:A:84:ASP:OD2	2.51	0.43
1:E:50:ILE:HA	1:E:55:ASN:O	2.19	0.43
1:C:141:PHE:HE1	1:C:175:MET:HA	1.83	0.43
1:C:56:ARG:HH21	1:C:62:ALA:C	2.21	0.43
1:A:95:SER:O	1:A:96:ASN:HB3	2.17	0.43
2:D:27:TYR:HE1	2:D:98:ARG:HD3	1.82	0.43
2:D:84:ASN:O	2:D:85:SER:C	2.56	0.43
1:C:136:CYS:HB2	1:C:150:TRP:CZ2	2.53	0.43
1:C:164:THR:CB	2:D:172:PRO:HG2	2.48	0.43
2:F:10:GLU:HG2	2:F:18:VAL:HG12	2.00	0.43
1:C:83:GLU:C	1:C:85:GLU:N	2.71	0.43
2:H:81:LEU:HD11	2:H:83:LEU:HD21	1.99	0.43
2:F:29:PHE:CE2	2:F:74:ARG:HA	2.53	0.43
2:D:159:TRP:CZ3	2:D:200:CYS:HB3	2.54	0.43
2:B:159:TRP:CZ3	2:B:200:CYS:HB3	2.53	0.43
1:A:72:LYS:HB2	1:A:72:LYS:HZ2	1.81	0.43
1:G:164:THR:CG2	1:G:177:SER:OG	2.66	0.43
1:G:64:PHE:CE1	1:G:77:ILE:HG12	2.53	0.43
2:D:23:ARG:HB3	2:D:78:ILE:HG12	1.99	0.43
2:H:32:TYR:O	2:H:53:PRO:HD2	2.19	0.43
2:D:35:GLN:HE22	2:D:98:ARG:C	2.21	0.43
2:H:174:VAL:CG2	2:H:181:THR:HG23	2.49	0.43
2:B:39:GLN:O	2:B:92:ALA:HB1	2.18	0.43
3:D:352:ECO:H192	3:D:352:ECO:HC71	2.01	0.43
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.99	0.43
2:D:52:TYR:HB3	2:D:57:ASP:HB3	1.99	0.43
2:H:11:LEU:HD13	2:H:12:ALA:N	2.34	0.43
2:B:143:LEU:N	2:B:143:LEU:HD22	2.33	0.43
2:F:111:GLN:NE2	2:F:112:GLY:N	2.66	0.43
2:D:27:TYR:CD1	2:D:98:ARG:NH1	2.86	0.43
1:A:152:VAL:HG12	1:A:190:HIS:CD2	2.54	0.43
1:A:152:VAL:HG22	1:A:193:TYR:HD2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:THR:OG1	2:B:29:PHE:HD1	2.02	0.43
1:A:63:ARG:CZ	1:A:81:GLN:CG	2.96	0.43
2:H:70:LEU:CD1	2:H:81:LEU:HD23	2.48	0.43
1:G:57:ALA:HB1	1:G:58:PRO:HD2	1.99	0.43
1:G:152:VAL:HG22	1:G:193:TYR:HD2	1.84	0.43
1:G:68:LEU:HD23	1:G:73:ALA:HA	2.01	0.43
1:A:146:VAL:HG12	1:A:199:HIS:HB2	2.01	0.43
1:G:23:ARG:NH2	1:G:72:LYS:CE	2.79	0.42
2:F:60:TYR:OH	2:F:69:THR:HA	2.18	0.42
1:E:161:MET:HA	1:E:179:TYR:O	2.19	0.42
1:A:93:TRP:HE3	1:A:98:PHE:CE1	2.37	0.42
2:B:36:TRP:NE1	2:B:70:LEU:HD11	2.33	0.42
1:A:61:PRO:O	1:A:63:ARG:N	2.52	0.42
1:E:88:TYR:HE2	1:E:106:VAL:HG21	1.83	0.42
2:H:57:ASP:CG	2:H:59:ARG:HH11	2.21	0.42
2:F:10:GLU:HG2	2:F:18:VAL:HG11	2.00	0.42
4:G:217:HOH:O	2:H:171:PHE:HB2	2.19	0.42
2:D:60:TYR:HE2	2:D:70:LEU:HD13	1.85	0.42
1:C:209:SER:O	1:C:210:ALA:C	2.58	0.42
2:B:23:ARG:HA	2:B:77:SER:O	2.19	0.42
1:C:30:THR:C	1:C:68:LEU:HD11	2.40	0.42
1:C:63:ARG:HB2	1:C:78:THR:O	2.19	0.42
1:E:49:LEU:HD12	1:E:49:LEU:HA	1.84	0.42
1:C:18:VAL:CG1	1:C:77:ILE:HD12	2.49	0.42
2:D:62:GLN:OE1	2:D:62:GLN:HA	2.19	0.42
1:E:130:ASN:HD22	1:E:130:ASN:HA	1.66	0.42
1:E:183:THR:O	1:E:184:ALA:C	2.58	0.42
1:C:57:ALA:HB3	1:C:60:VAL:CG2	2.50	0.42
2:F:33:TRP:O	2:F:34:MET:HB2	2.20	0.42
1:C:20:LEU:N	1:C:20:LEU:HD12	2.34	0.42
1:E:53:THR:HG23	1:E:68:LEU:HG	2.02	0.42
1:C:96:ASN:HA	3:D:352:ECO:C3	2.49	0.42
2:B:48:ILE:HG12	2:B:64:PHE:CE2	2.54	0.42
2:B:122:THR:HG21	2:B:179:LEU:HD21	2.01	0.42
1:A:115:PRO:HA	1:A:139:THR:O	2.20	0.42
1:E:72:LYS:N	1:E:72:LYS:HD3	2.35	0.42
1:C:19:THR:HA	1:C:75:LEU:O	2.19	0.42
1:C:4:VAL:HG12	1:C:5:THR:N	2.34	0.42
2:B:51:ILE:O	2:B:53:PRO:HD3	2.20	0.42
1:G:34:TYR:O	1:G:35:ALA:C	2.57	0.42
2:H:45:LEU:HG	4:H:357:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:HB	2:B:171:PHE:CZ	2.54	0.42
1:C:93:TRP:NE1	2:D:102:LEU:CD1	2.83	0.42
1:C:22:CYS:HB3	1:C:73:ALA:HB3	2.01	0.42
1:C:208:LEU:O	1:C:208:LEU:HD12	2.19	0.42
1:A:174:TYR:CD1	1:A:174:TYR:N	2.88	0.42
1:E:4:VAL:HA	1:E:23:ARG:O	2.20	0.42
1:E:175:MET:HE1	2:F:169:HIS:ND1	2.35	0.42
1:E:96:ASN:HA	3:F:353:ECO:C2	2.49	0.42
1:G:51:SER:O	1:G:55:ASN:HB2	2.20	0.42
1:G:101:GLY:C	1:G:103:GLY:H	2.23	0.42
1:G:174:TYR:CD1	1:G:174:TYR:N	2.87	0.42
2:B:34:MET:HG2	2:B:79:VAL:HG11	2.01	0.42
2:D:27:TYR:CE1	2:D:98:ARG:HD3	2.55	0.42
2:D:122:THR:HG21	2:D:179:LEU:HD21	2.01	0.42
1:E:136:CYS:HB2	1:E:150:TRP:CZ2	2.55	0.42
1:A:69:ILE:O	1:A:72:LYS:NZ	2.53	0.41
2:H:175:LEU:HD13	2:H:180:TYR:CZ	2.55	0.41
2:F:194:PRO:O	2:F:195:SER:C	2.58	0.41
1:E:2:ALA:HB1	1:E:26:SER:H	1.85	0.41
1:C:141:PHE:CE1	1:C:175:MET:HA	2.55	0.41
1:A:152:VAL:O	1:A:153:ASP:HB2	2.20	0.41
1:A:193:TYR:O	1:A:207:SER:HA	2.20	0.41
2:H:37:VAL:CG1	2:H:45:LEU:HB3	2.51	0.41
2:D:37:VAL:CG1	2:D:45:LEU:HB3	2.51	0.41
2:D:150:TYR:CE1	2:D:155:VAL:HG13	2.55	0.41
2:D:86:LEU:HD12	2:D:90:ASP:CB	2.50	0.41
1:G:56:ARG:CB	1:G:56:ARG:HH11	2.32	0.41
1:C:151:LYS:HB2	1:C:194:SER:HB3	2.02	0.41
2:B:105:THR:O	2:B:106:MET:HB2	2.20	0.41
1:A:34:TYR:CD1	2:B:102:LEU:HD13	2.55	0.41
1:C:134:LEU:HD11	1:C:187:TRP:CZ3	2.54	0.41
1:E:38:ILE:CG2	1:E:46:PHE:HB3	2.50	0.41
3:B:351:ECO:O3	2:F:56:ASP:HB2	2.19	0.41
1:C:30:THR:HA	1:C:68:LEU:CD1	2.51	0.41
2:D:48:ILE:HA	2:D:64:PHE:CE2	2.55	0.41
2:F:33:TRP:HB3	2:F:34:MET:H	1.58	0.41
1:E:16:GLU:HB3	1:E:17:THR:H	1.74	0.41
2:F:13:ARG:HE	2:F:13:ARG:CA	2.34	0.41
1:E:6:GLN:HB3	1:E:7:GLU:H	1.57	0.41
2:D:57:ASP:CG	2:D:59:ARG:HE	2.22	0.41
1:C:164:THR:HB	2:D:172:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:HIS:HD2	2:H:207:SER:OG	2.04	0.41
1:E:29:ILE:O	1:E:68:LEU:HD22	2.21	0.41
2:D:174:VAL:CG2	2:D:181:THR:HG23	2.51	0.41
2:H:143:LEU:HB3	2:H:215:ILE:HG12	2.03	0.41
1:C:152:VAL:CG1	1:C:190:HIS:CD2	3.03	0.41
1:A:6:GLN:HB3	1:A:104:THR:OG1	2.20	0.41
2:H:38:ARG:HG3	2:H:38:ARG:O	2.19	0.41
1:G:136:CYS:HB2	1:G:150:TRP:CZ2	2.56	0.41
2:B:4:LEU:O	2:B:110:GLY:HA2	2.20	0.41
3:F:353:ECO:H192	3:F:353:ECO:C7	2.51	0.41
1:C:12:THR:HG23	1:C:108:VAL:HG22	2.02	0.41
2:D:81:LEU:CD2	2:D:82:GLN:N	2.84	0.41
1:C:93:TRP:HE3	1:C:93:TRP:HA	1.85	0.41
1:E:34:TYR:HB3	2:F:102:LEU:O	2.21	0.41
2:H:4:LEU:HA	2:H:23:ARG:O	2.21	0.41
2:D:55:ASP:OD2	2:H:60:TYR:N	2.54	0.41
1:C:64:PHE:HZ	1:C:88:TYR:HH	1.65	0.41
2:D:28:SER:HB2	2:D:31:THR:HG23	2.02	0.41
1:E:117:VAL:HG11	1:E:206:LYS:HB2	2.02	0.41
1:E:29:ILE:O	1:E:68:LEU:HD13	2.21	0.40
1:C:18:VAL:HG12	1:C:77:ILE:HB	2.02	0.40
1:A:23:ARG:NH1	1:A:23:ARG:CB	2.84	0.40
2:D:44:GLY:N	4:D:354:HOH:O	2.54	0.40
1:E:29:ILE:HD13	1:E:72:LYS:HA	2.02	0.40
1:E:93:TRP:NE1	1:E:95:SER:HA	2.36	0.40
2:F:37:VAL:CG1	2:F:46:GLU:O	2.66	0.40
1:A:179:TYR:OH	2:B:183:SER:HB2	2.21	0.40
1:E:145:VAL:HG13	1:E:145:VAL:O	2.21	0.40
2:F:6:GLN:HE21	2:F:110:GLY:HA3	1.87	0.40
1:E:18:VAL:HG22	1:E:19:THR:H	1.85	0.40
1:E:2:ALA:HA	1:E:25:SER:HB3	2.04	0.40
2:B:55:ASP:O	2:B:55:ASP:OD2	2.39	0.40
1:G:56:ARG:CZ	1:G:56:ARG:HB2	2.51	0.40
1:E:63:ARG:CZ	1:E:81:GLN:HG3	2.51	0.40
1:E:152:VAL:O	1:E:153:ASP:HB2	2.20	0.40
2:H:67:LYS:HB3	2:H:67:LYS:NZ	2.37	0.40
2:H:4:LEU:HD22	2:H:24:THR:HG22	2.02	0.40
1:G:4:VAL:HG23	1:G:99:ILE:HG22	2.03	0.40
1:G:1:GLN:HB3	1:G:99:ILE:HD11	2.03	0.40
2:H:76:SER:O	2:H:77:SER:HB2	2.21	0.40
2:H:174:VAL:HG22	2:H:181:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:THR:HA	1:G:178:SER:HA	2.04	0.40
2:H:69:THR:C	2:H:70:LEU:HD12	2.42	0.40
1:C:38:ILE:HD13	2:D:109:TRP:CZ2	2.56	0.40
1:C:41:LYS:O	1:C:42:PRO:C	2.60	0.40
1:E:182:LEU:HD11	1:E:193:TYR:CE2	2.56	0.40
1:A:194:SER:HB2	1:A:207:SER:OG	2.21	0.40
1:A:96:ASN:O	1:A:97:GLN:HB3	2.20	0.40
1:A:30:THR:HG1	1:A:32:SER:HG	1.70	0.40
1:C:183:THR:O	1:C:184:ALA:C	2.60	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	204/212 (96%)	180 (88%)	17 (8%)	7 (3%)	5	16
1	C	204/212 (96%)	174 (85%)	17 (8%)	13 (6%)	2	4
1	E	204/212 (96%)	167 (82%)	24 (12%)	13 (6%)	2	4
1	G	204/212 (96%)	179 (88%)	19 (9%)	6 (3%)	6	20
2	B	210/218 (96%)	180 (86%)	23 (11%)	7 (3%)	5	17
2	D	210/218 (96%)	179 (85%)	25 (12%)	6 (3%)	6	20
2	F	210/218 (96%)	184 (88%)	21 (10%)	5 (2%)	7	25
2	H	210/218 (96%)	183 (87%)	23 (11%)	4 (2%)	10	32
All	All	1656/1720 (96%)	1426 (86%)	169 (10%)	61 (4%)	4	14

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU

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Mol	Chain	Res	Type
1	A	95	SER
2	B	41	PRO
2	B	55	ASP
2	B	56	ASP
1	C	145	VAL
2	D	41	PRO
1	E	95	SER
2	F	41	PRO
1	G	95	SER
1	G	145	VAL
2	H	41	PRO
1	A	145	VAL
2	B	44	GLY
1	C	54	ASN
1	C	95	SER
1	C	96	ASN
1	C	210	ALA
2	D	44	GLY
2	D	55	ASP
1	E	2	ALA
1	E	16	GLU
1	E	35	ALA
1	E	145	VAL
2	F	9	ALA
2	F	34	MET
2	F	55	ASP
2	H	55	ASP
1	A	62	ALA
2	B	42	GLY
2	D	27	TYR
1	E	80	ALA
1	E	164	THR
2	H	25	SER
2	H	67	LYS
1	A	34	TYR
2	B	16	ALA
1	C	80	ALA
1	E	34	TYR
1	E	210	ALA
1	G	16	GLU
1	G	43	ASP
1	C	35	ALA

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Mol	Chain	Res	Type
1	C	58	PRO
1	C	59	GLY
1	C	185	ARG
2	D	62	GLN
2	D	195	SER
1	E	31	THR
1	E	185	ARG
2	F	44	GLY
1	G	97	GLN
1	G	164	THR
1	A	43	ASP
1	A	96	ASN
2	B	28	SER
1	C	26	SER
1	C	34	TYR
1	C	42	PRO
1	E	42	PRO
1	E	79	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	176/180 (98%)	166 (94%)	10 (6%)	25	56
1	C	176/180 (98%)	165 (94%)	11 (6%)	22	50
1	E	176/180 (98%)	167 (95%)	9 (5%)	29	62
1	G	176/180 (98%)	162 (92%)	14 (8%)	15	38
2	B	178/187 (95%)	152 (85%)	26 (15%)	4	10
2	D	178/187 (95%)	153 (86%)	25 (14%)	4	11
2	F	178/187 (95%)	157 (88%)	21 (12%)	6	17
2	H	178/187 (95%)	151 (85%)	27 (15%)	3	9
All	All	1416/1468 (96%)	1273 (90%)	143 (10%)	9	25

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	47	THR
1	A	78	THR
1	A	96	ASN
1	A	119	LEU
1	A	124	SER
1	A	148	VAL
1	A	185	ARG
1	A	202	HIS
1	A	208	LEU
2	B	1	GLU
2	B	11	LEU
2	B	13	ARG
2	B	22	CYS
2	B	32	TYR
2	B	41	PRO
2	B	67	LYS
2	B	69	THR
2	B	81	LEU
2	B	86	LEU
2	B	89	GLU
2	B	96	CYS
2	B	111	GLN
2	B	113	THR
2	B	121	THR
2	B	122	THR
2	B	142	THR
2	B	143	LEU
2	B	145	CYS
2	B	152	PRO
2	B	154	PRO
2	B	164	LEU
2	B	181	THR
2	B	182	LEU
2	B	201	ASN
2	B	215	ILE
1	C	6	GLN
1	C	45	LEU
1	C	56	ARG
1	C	76	THR
1	C	96	ASN
1	C	119	LEU
1	C	124	SER

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Mol	Chain	Res	Type
1	C	148	VAL
1	C	185	ARG
1	C	202	HIS
1	C	208	LEU
2	D	1	GLU
2	D	10	GLU
2	D	13	ARG
2	D	27	TYR
2	D	41	PRO
2	D	55	ASP
2	D	59	ARG
2	D	71	THR
2	D	81	LEU
2	D	86	LEU
2	D	96	CYS
2	D	111	GLN
2	D	121	THR
2	D	122	THR
2	D	142	THR
2	D	143	LEU
2	D	145	CYS
2	D	152	PRO
2	D	154	PRO
2	D	164	LEU
2	D	181	THR
2	D	182	LEU
2	D	200	CYS
2	D	201	ASN
2	D	215	ILE
1	E	11	THR
1	E	20	LEU
1	E	36	ASN
1	E	72	LYS
1	E	119	LEU
1	E	124	SER
1	E	148	VAL
1	E	202	HIS
1	E	208	LEU
2	F	1	GLU
2	F	11	LEU
2	F	13	ARG
2	F	18	VAL

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Mol	Chain	Res	Type
2	F	41	PRO
2	F	59	ARG
2	F	67	LYS
2	F	81	LEU
2	F	96	CYS
2	F	121	THR
2	F	122	THR
2	F	142	THR
2	F	143	LEU
2	F	145	CYS
2	F	154	PRO
2	F	164	LEU
2	F	181	THR
2	F	182	LEU
2	F	200	CYS
2	F	201	ASN
2	F	215	ILE
1	G	20	LEU
1	G	25	SER
1	G	30	THR
1	G	36	ASN
1	G	45	LEU
1	G	47	THR
1	G	96	ASN
1	G	119	LEU
1	G	124	SER
1	G	148	VAL
1	G	162	GLU
1	G	185	ARG
1	G	202	HIS
1	G	208	LEU
2	H	3	GLN
2	H	4	LEU
2	H	10	GLU
2	H	11	LEU
2	H	13	ARG
2	H	22	CYS
2	H	31	THR
2	H	35	GLN
2	H	41	PRO
2	H	55	ASP
2	H	59	ARG

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Mol	Chain	Res	Type
2	H	60	TYR
2	H	67	LYS
2	H	96	CYS
2	H	111	GLN
2	H	113	THR
2	H	122	THR
2	H	142	THR
2	H	143	LEU
2	H	145	CYS
2	H	154	PRO
2	H	164	LEU
2	H	181	THR
2	H	182	LEU
2	H	200	CYS
2	H	201	ASN
2	H	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	36	ASN
1	A	96	ASN
1	A	97	GLN
1	A	130	ASN
1	A	202	HIS
2	B	3	GLN
2	B	6	GLN
2	B	35	GLN
2	B	39	GLN
2	B	43	GLN
2	B	82	GLN
2	B	84	ASN
2	B	111	GLN
2	B	204	HIS
1	C	1	GLN
1	C	39	GLN
1	C	54	ASN
1	C	130	ASN
2	D	6	GLN
2	D	35	GLN
2	D	39	GLN

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Mol	Chain	Res	Type
2	D	43	GLN
2	D	82	GLN
2	D	111	GLN
2	D	176	GLN
2	D	204	HIS
1	E	1	GLN
1	E	6	GLN
1	E	36	ASN
1	E	130	ASN
1	E	196	GLN
1	E	202	HIS
2	F	3	GLN
2	F	6	GLN
2	F	35	GLN
2	F	39	GLN
2	F	43	GLN
2	F	111	GLN
2	F	204	HIS
1	G	1	GLN
1	G	36	ASN
1	G	96	ASN
1	G	130	ASN
2	H	3	GLN
2	H	6	GLN
2	H	35	GLN
2	H	39	GLN
2	H	43	GLN
2	H	82	GLN
2	H	111	GLN
2	H	204	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ECO	B	351	-	26,29,29	3.58	17 (65%)	38,44,44	2.56	8 (21%)
3	ECO	D	352	-	26,29,29	3.71	17 (65%)	38,44,44	2.59	7 (18%)
3	ECO	F	353	-	26,29,29	3.89	18 (69%)	38,44,44	2.59	3 (7%)
3	ECO	H	354	-	26,29,29	3.60	19 (73%)	38,44,44	2.52	7 (18%)

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
3	ECO	B	351	-	-	1/4/49/49	0/4/4/4
3	ECO	D	352	-	-	1/4/49/49	0/4/4/4
3	ECO	F	353	-	-	1/4/49/49	0/4/4/4
3	ECO	H	354	-	-	1/4/49/49	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	354	ECO	O19-C19	-2.60	1.40	1.44
3	F	353	ECO	O19-C19	-2.53	1.40	1.44
3	B	351	ECO	O19-C19	-2.28	1.40	1.44
3	H	354	ECO	C13-C17	2.13	1.57	1.54
3	H	354	ECO	C10-C9	2.25	1.55	1.52
3	D	352	ECO	C16-C17	2.26	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	351	ECO	C2-C1	2.33	1.42	1.38
3	B	351	ECO	C2-C3	2.35	1.43	1.38
3	F	353	ECO	C16-C17	2.35	1.57	1.53
3	B	351	ECO	C16-C17	2.42	1.57	1.53
3	D	352	ECO	C10-C9	2.44	1.56	1.52
3	H	354	ECO	C2-C3	2.57	1.44	1.38
3	H	354	ECO	C2-C1	2.58	1.43	1.38
3	D	352	ECO	C11-C9	2.67	1.57	1.53
3	H	354	ECO	O19-N19	2.68	1.47	1.42
3	H	354	ECO	C16-C17	2.70	1.58	1.53
3	D	352	ECO	C2-C1	2.75	1.43	1.38
3	D	352	ECO	C2-C3	2.77	1.44	1.38
3	H	354	ECO	C4-C3	2.90	1.43	1.39
3	B	351	ECO	C4-C3	2.96	1.43	1.39
3	F	353	ECO	C10-C9	3.02	1.57	1.52
3	F	353	ECO	C2-C1	3.05	1.44	1.38
3	D	352	ECO	C13-C14	3.07	1.61	1.55
3	F	353	ECO	C2-C3	3.07	1.45	1.38
3	H	354	ECO	C18-C13	3.10	1.60	1.54
3	B	351	ECO	C5-C6	3.14	1.55	1.47
3	H	354	ECO	C11-C9	3.16	1.58	1.53
3	H	354	ECO	C8-C14	3.17	1.59	1.53
3	B	351	ECO	C18-C13	3.18	1.60	1.54
3	B	351	ECO	O19-N19	3.26	1.48	1.42
3	F	353	ECO	O19-N19	3.28	1.48	1.42
3	D	352	ECO	C8-C14	3.29	1.60	1.53
3	B	351	ECO	C8-C14	3.30	1.60	1.53
3	F	353	ECO	C4-C3	3.31	1.44	1.39
3	H	354	ECO	C5-C6	3.35	1.55	1.47
3	F	353	ECO	C8-C14	3.36	1.60	1.53
3	B	351	ECO	C13-C14	3.39	1.61	1.55
3	B	351	ECO	C4-C5	3.42	1.45	1.39
3	F	353	ECO	C13-C14	3.43	1.61	1.55
3	F	353	ECO	C11-C9	3.45	1.58	1.53
3	D	352	ECO	C5-C6	3.49	1.56	1.47
3	D	352	ECO	O19-N19	3.50	1.49	1.42
3	F	353	ECO	C18-C13	3.52	1.60	1.54
3	D	352	ECO	C18-C13	3.60	1.61	1.54
3	B	351	ECO	C11-C9	3.61	1.58	1.53
3	F	353	ECO	C5-C6	3.63	1.56	1.47
3	D	352	ECO	C4-C3	3.74	1.45	1.39
3	H	354	ECO	C7-C6	3.78	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	354	ECO	C13-C14	3.84	1.62	1.55
3	H	354	ECO	C4-C5	3.86	1.46	1.39
3	B	351	ECO	C7-C6	3.87	1.59	1.50
3	D	352	ECO	C7-C6	3.87	1.59	1.50
3	D	352	ECO	C4-C5	3.92	1.46	1.39
3	F	353	ECO	C4-C5	3.95	1.46	1.39
3	F	353	ECO	C7-C6	4.11	1.59	1.50
3	B	351	ECO	C1-C10	4.15	1.45	1.39
3	H	354	ECO	C1-C10	4.53	1.45	1.39
3	D	352	ECO	C1-C10	5.17	1.46	1.39
3	F	353	ECO	C1-C10	5.29	1.47	1.39
3	B	351	ECO	C9-C8	5.33	1.60	1.54
3	H	354	ECO	C9-C8	5.46	1.60	1.54
3	D	352	ECO	C9-C8	5.55	1.60	1.54
3	F	353	ECO	C9-C8	6.22	1.61	1.54
3	B	351	ECO	C5-C10	7.19	1.49	1.40
3	H	354	ECO	C5-C10	7.74	1.49	1.40
3	D	352	ECO	C5-C10	7.80	1.49	1.40
3	F	353	ECO	C5-C10	7.91	1.49	1.40
3	H	354	ECO	C6-N19	9.00	1.37	1.28
3	D	352	ECO	C6-N19	9.66	1.38	1.28
3	F	353	ECO	C6-N19	9.78	1.38	1.28
3	B	351	ECO	C6-N19	10.10	1.38	1.28

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	352	ECO	C15-C14-C13	-2.91	100.03	103.82
3	B	351	ECO	C15-C14-C13	-2.59	100.45	103.82
3	B	351	ECO	C7-C6-C5	-2.55	113.33	118.91
3	D	352	ECO	C11-C9-C8	-2.55	107.80	111.30
3	B	351	ECO	C5-C6-N19	-2.48	113.58	116.92
3	D	352	ECO	C7-C6-C5	-2.41	113.63	118.91
3	F	353	ECO	C15-C14-C13	-2.34	100.78	103.82
3	H	354	ECO	C15-C14-C13	-2.32	100.81	103.82
3	H	354	ECO	C7-C6-C5	-2.25	113.98	118.91
3	B	351	ECO	C11-C9-C8	-2.18	108.31	111.30
3	F	353	ECO	C13-C14-C8	-2.16	110.99	114.37
3	H	354	ECO	C11-C9-C8	-2.04	108.50	111.30
3	B	351	ECO	C12-C11-C9	2.00	114.54	112.20
3	D	352	ECO	C15-C14-C8	2.00	122.19	119.03
3	B	351	ECO	C16-C17-C13	2.12	106.22	104.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	354	ECO	C12-C11-C9	2.15	114.72	112.20
3	H	354	ECO	C16-C17-C13	2.16	106.25	104.58
3	B	351	ECO	C8-C7-C6	2.17	113.91	111.08
3	H	354	ECO	C8-C7-C6	2.18	113.92	111.08
3	D	352	ECO	C16-C17-C13	2.20	106.29	104.58
3	D	352	ECO	C8-C7-C6	2.29	114.06	111.08
3	B	351	ECO	C19-O19-N19	13.45	123.65	108.00
3	H	354	ECO	C19-O19-N19	13.49	123.69	108.00
3	D	352	ECO	C19-O19-N19	13.68	123.91	108.00
3	F	353	ECO	C19-O19-N19	14.10	124.40	108.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	351	ECO	C19-O19-N19-C6
3	D	352	ECO	C19-O19-N19-C6
3	F	353	ECO	C19-O19-N19-C6
3	H	354	ECO	C19-O19-N19-C6

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	351	ECO	3	0
3	D	352	ECO	3	0
3	F	353	ECO	3	0
3	H	354	ECO	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/212 (98%)	-0.10	4 (1%) 70 66	15, 55, 103, 150	0
1	C	208/212 (98%)	0.21	12 (5%) 26 20	11, 74, 123, 155	0
1	E	208/212 (98%)	0.53	31 (14%) 3 2	11, 82, 138, 191	0
1	G	208/212 (98%)	-0.20	2 (0%) 84 81	17, 46, 101, 148	0
2	B	214/218 (98%)	-0.27	1 (0%) 91 90	18, 45, 90, 117	0
2	D	214/218 (98%)	-0.20	2 (0%) 85 84	13, 47, 98, 134	0
2	F	214/218 (98%)	-0.16	1 (0%) 91 90	12, 51, 105, 156	0
2	H	214/218 (98%)	-0.28	1 (0%) 91 90	13, 40, 88, 129	0
All	All	1688/1720 (98%)	-0.06	54 (3%) 51 44	11, 51, 116, 191	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	86	ALA	5.3
1	E	10	LEU	5.1
1	E	79	GLY	4.7
1	E	171	ASN	4.4
1	E	77	ILE	4.1
1	E	12	THR	4.0
1	E	2	ALA	3.5
1	E	38	ILE	3.3
1	E	211	ALA	3.2
1	E	23	ARG	3.1
1	E	1	GLN	3.1
1	C	77	ILE	3.0
1	E	24	SER	3.0
1	C	18	VAL	3.0
1	E	88	TYR	3.0
1	E	21	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	78	THR	2.9
1	E	108	VAL	2.8
1	C	86	ALA	2.8
1	E	61	PRO	2.8
1	A	80	ALA	2.7
1	E	65	SER	2.6
1	E	87	ILE	2.6
1	G	172	ASN	2.6
1	E	66	GLY	2.5
1	E	106	VAL	2.5
1	C	58	PRO	2.5
1	C	50	ILE	2.4
1	C	82	THR	2.4
1	C	171	ASN	2.4
2	D	96	CYS	2.4
2	H	138	ASN	2.4
1	E	68	LEU	2.3
1	E	15	GLY	2.3
1	E	20	LEU	2.3
1	C	78	THR	2.3
1	C	64	PHE	2.3
1	C	12	THR	2.2
2	F	15	GLY	2.2
1	A	108	VAL	2.2
2	B	136	GLN	2.2
1	E	75	LEU	2.2
1	E	81	GLN	2.1
1	C	49	LEU	2.1
1	E	64	PHE	2.1
1	G	142	TYR	2.1
1	C	108	VAL	2.1
1	A	170	SER	2.1
1	A	142	TYR	2.1
1	E	104	THR	2.1
1	E	19	THR	2.0
2	D	43	GLN	2.0
1	E	49	LEU	2.0
1	E	9	ALA	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
3	ECO	H	354	26/26	0.87	0.23	2.97	52,53,88,88	0
3	ECO	B	351	26/26	0.88	0.21	1.36	52,53,88,88	0
3	ECO	F	353	26/26	0.84	0.20	0.76	52,53,88,88	0
3	ECO	D	352	26/26	0.89	0.22	0.54	52,53,88,88	0

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

There are no such residues in this entry.