



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:30 PM GMT

PDB ID : 1E79
Title : Bovine F1-ATPase inhibited by DCCD (dicyclohexylcarbodiimide)
Authors : Gibbons, C.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2000-08-25
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

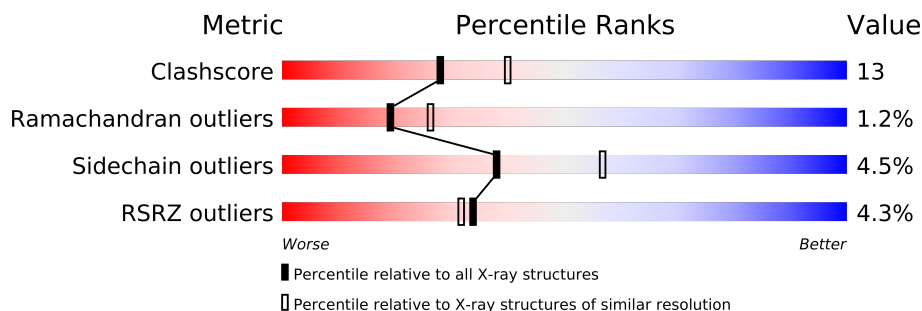
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	
4	H	146	
5	I	50	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	DCW	D	700	-	X
11	SO4	E	630	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
7	MG	C	601	-	X
7	MG	D	601	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26318 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP SYNTHASE ALPHA CHAIN HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CLONING ARTIFACT	UNP P19483
B	481	GLY	SER	CLONING ARTIFACT	UNP P19483
C	481	GLY	SER	CLONING ARTIFACT	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3538	2243	601	683	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

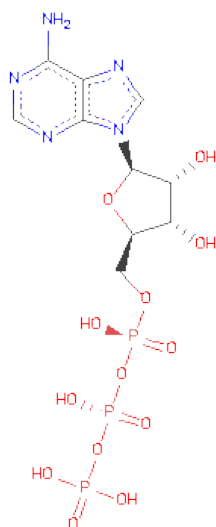
- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

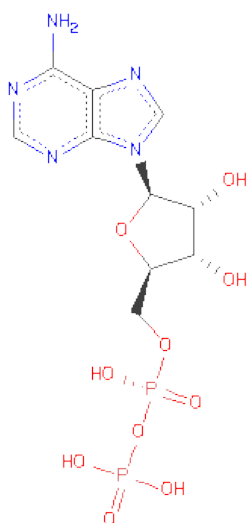
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



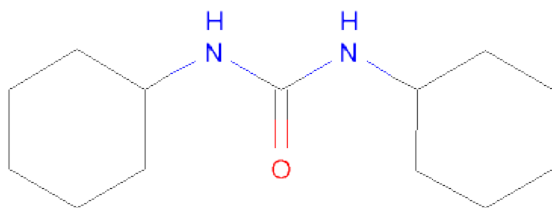
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



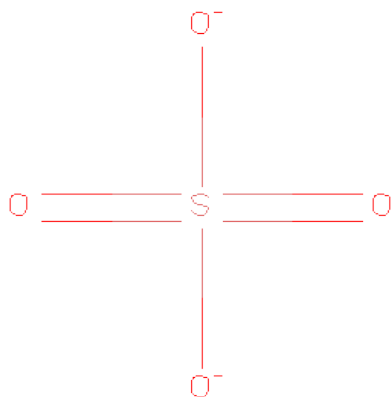
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is DICYCLOHEXYLUREA (three-letter code: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is water.

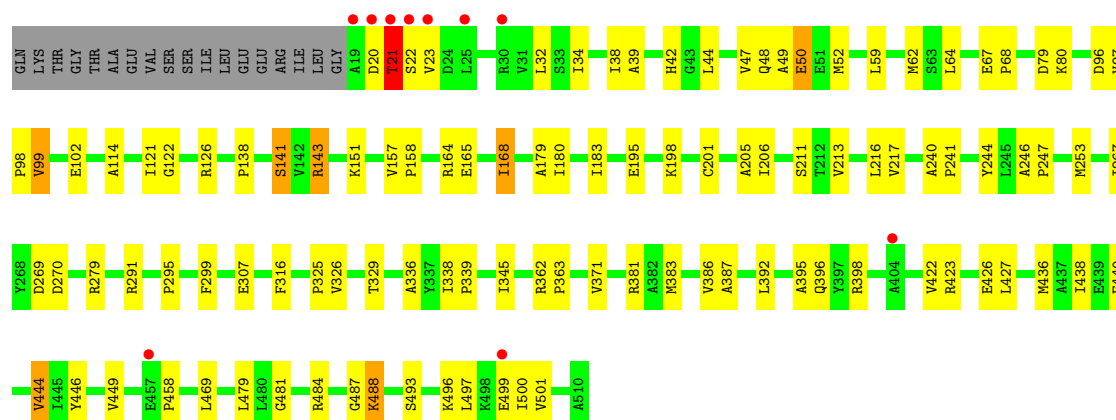
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	163	Total	O	0	0
			163	163		
12	B	140	Total	O	0	0
			140	140		
12	C	167	Total	O	0	0
			167	167		
12	D	148	Total	O	0	0
			148	148		
12	E	95	Total	O	0	0
			95	95		
12	F	164	Total	O	0	0
			164	164		
12	G	25	Total	O	0	0
			25	25		
12	H	5	Total	O	0	0
			5	5		
12	I	4	Total	O	0	0
			4	4		

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.

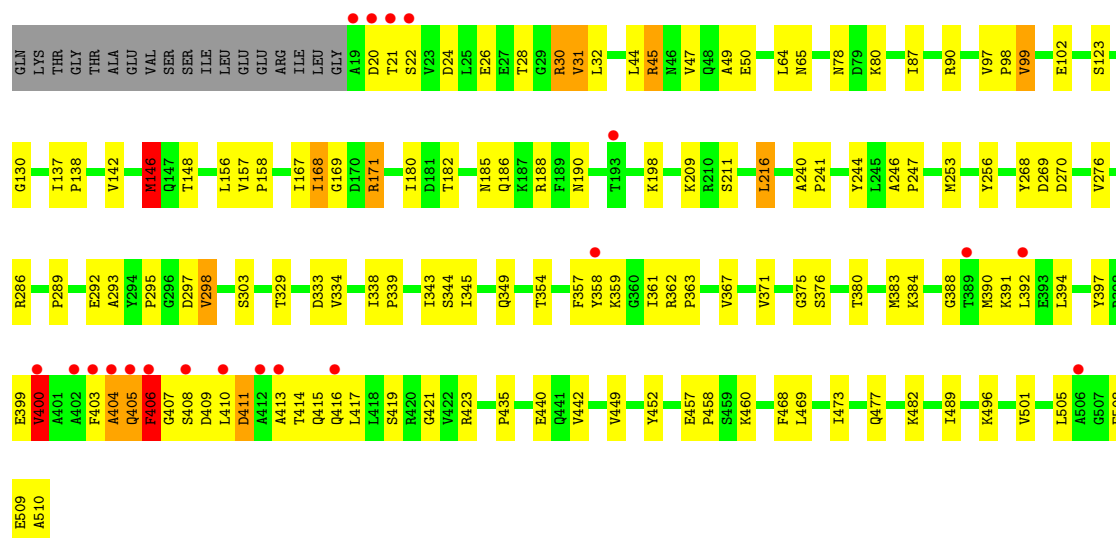
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM

Chain A: 



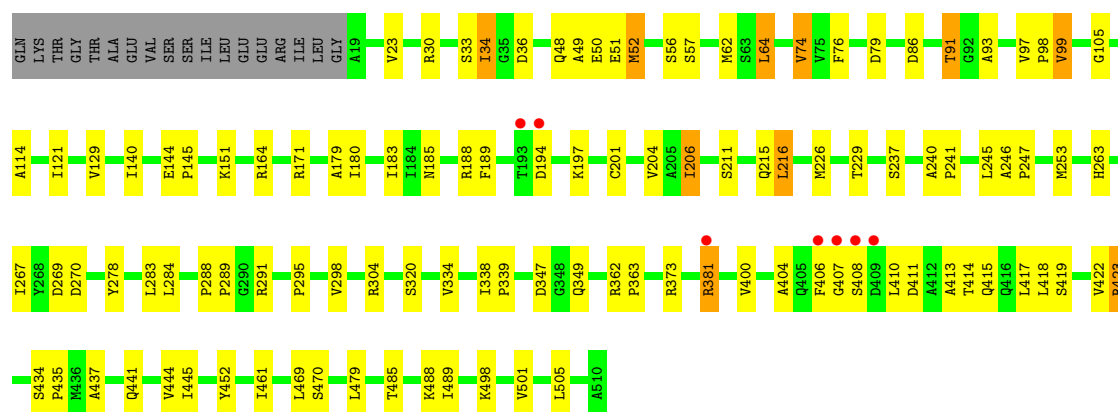
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM

Chain B: 



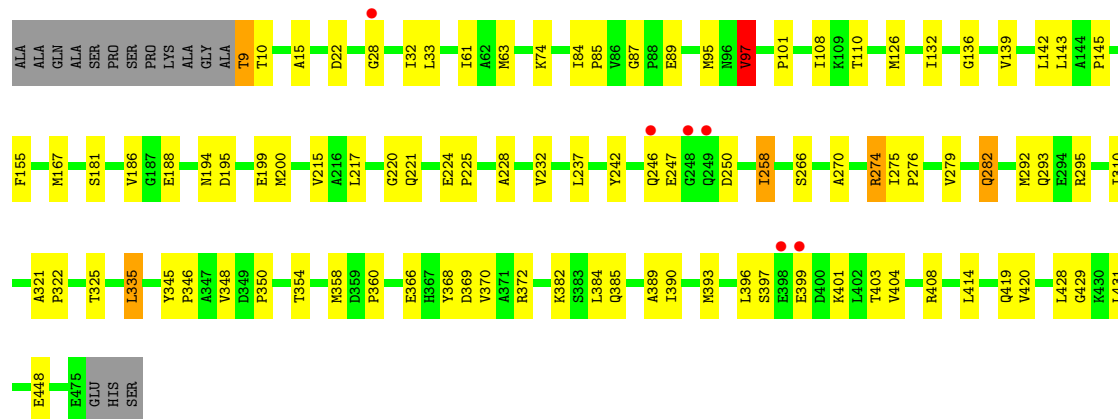
• Molecule 1: ATP SYNTHASE ALPHA CHAIN HEART ISOFORM

Chain C: 



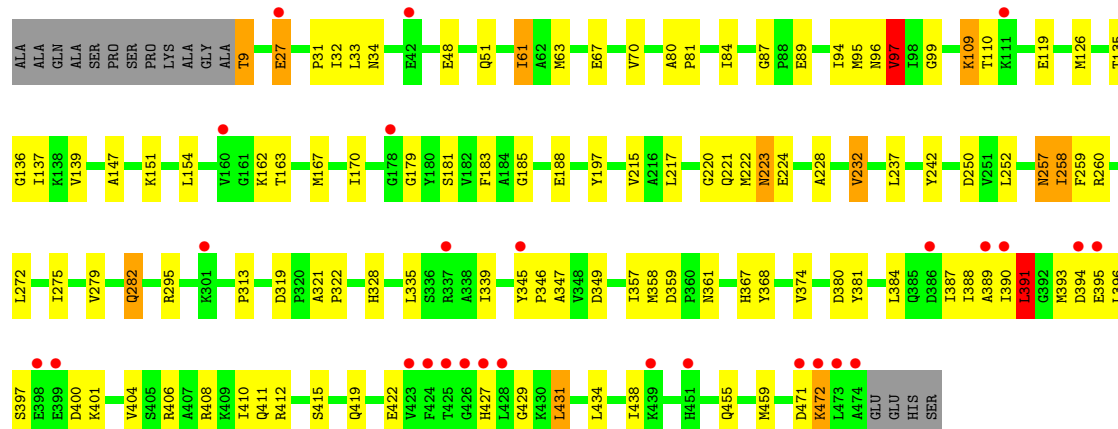
• Molecule 2: ATP SYNTHASE BETA CHAIN

Chain D:



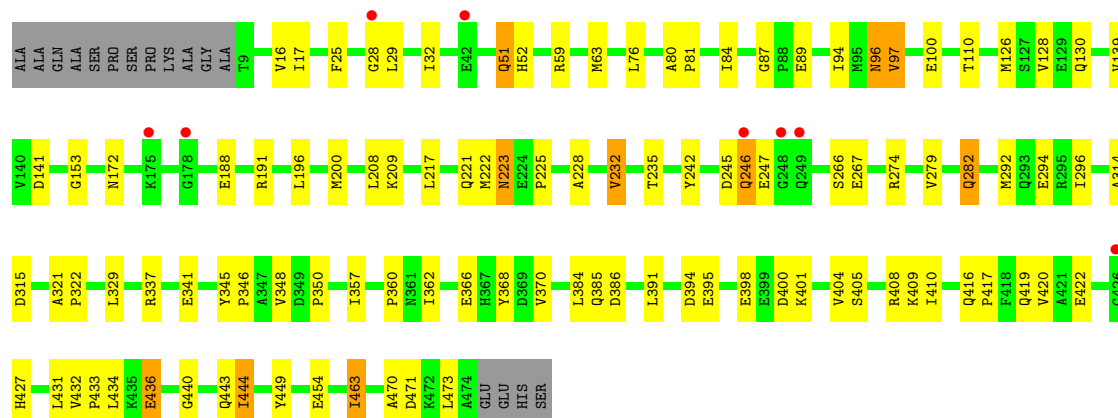
• Molecule 2: ATP SYNTHASE BETA CHAIN

Chain E:



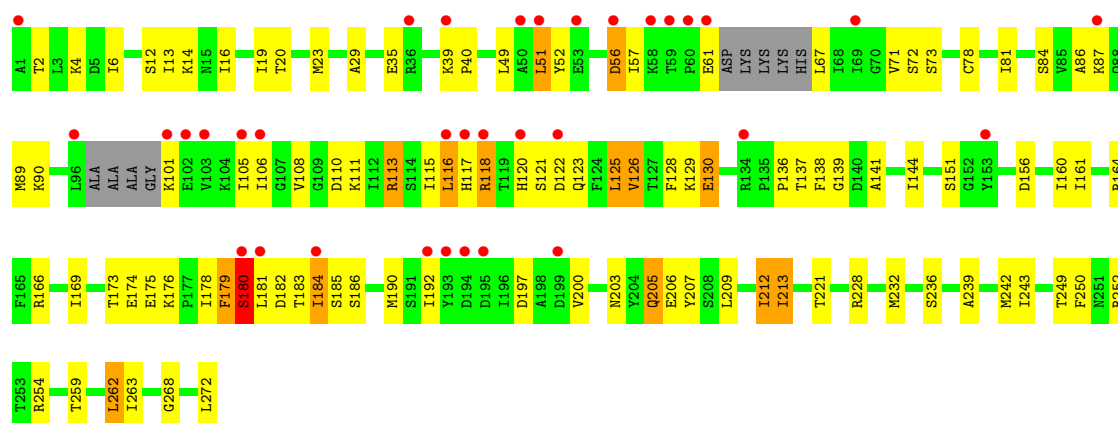
• Molecule 2: ATP SYNTHASE BETA CHAIN

Chain F:



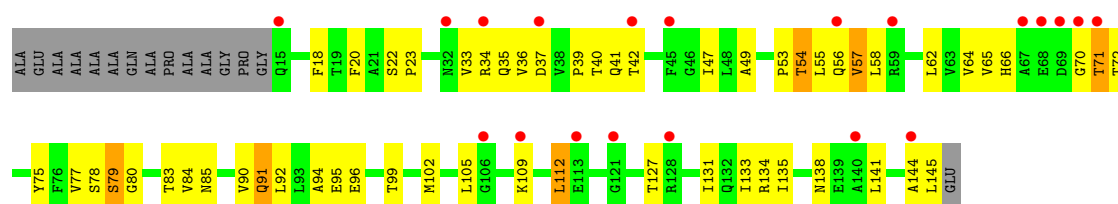
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain G:



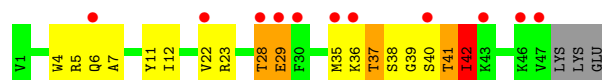
• Molecule 4: ATP SYNTHASE DELTA CHAIN

Chain H:



• Molecule 5: ATP SYNTHASE EPSILON CHAIN

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	267.20Å 107.20Å 135.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.2 (20.00-2.40) 91.9 (19.98-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.281 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 140093 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26318	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ADP, SO4, ATP, DCW

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	0.39	0/3799	0.78	0/5126
1	B	0.39	0/3799	0.81	2/5126 (0.0%)
1	C	0.40	0/3799	0.81	2/5126 (0.0%)
2	D	0.40	0/3595	0.81	2/4877 (0.0%)
2	E	0.38	0/3587	0.76	1/4867 (0.0%)
2	F	0.39	0/3587	0.79	1/4867 (0.0%)
3	G	0.35	0/2074	0.72	2/2785 (0.1%)
4	H	0.33	0/982	0.67	0/1337
5	I	0.34	0/374	0.71	0/501
All	All	0.38	0/25596	0.78	10/34612 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	195	ASP	N-CA-CB	8.67	126.21	110.60
1	B	45	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	F	191	ARG	NE-CZ-NH2	-6.49	117.06	120.30
3	G	254	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	423	ARG	CD-NE-CZ	5.33	131.06	123.60
1	B	146	MET	CG-SD-CE	5.20	108.51	100.20
2	E	97	VAL	CB-CA-C	-5.18	101.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	254	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	D	97	VAL	CB-CA-C	-5.14	101.62	111.40
1	C	291	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	194	ASN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3844	76	0
1	B	3748	0	3844	106	0
1	C	3748	0	3844	75	0
2	D	3538	0	3592	83	0
2	E	3530	0	3587	89	0
2	F	3530	0	3586	88	0
3	G	2051	0	2115	108	0
4	H	970	0	972	55	0
5	I	369	0	395	20	0
6	A	31	0	12	0	0
6	C	31	0	12	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	27	0	12	0	0
8	D	27	0	12	0	0
8	F	27	0	12	0	0
9	B	6	0	8	1	0
10	D	16	0	23	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	E	5	0	0	0	0
12	A	163	0	0	4	0
12	B	140	0	0	3	0
12	C	167	0	0	2	0
12	D	148	0	0	9	0
12	E	95	0	0	0	0
12	F	164	0	0	4	0
12	G	25	0	0	1	0
12	H	5	0	0	0	0
12	I	4	0	0	0	0
All	All	26318	0	25870	651	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (651) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:199:GLU:HG2	10:D:700:DCW:H71C	1.32	1.08
2:D:199:GLU:CG	10:D:700:DCW:H71C	1.85	1.06
3:G:90:LYS:HB3	3:G:116:LEU:HD11	1.38	1.01
1:B:406:PHE:HB2	1:B:409:ASP:HB2	1.44	1.00
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.98
2:E:181:SER:HB2	2:E:215:VAL:HG12	1.45	0.96
4:H:62:LEU:HD11	4:H:144:ALA:HB2	1.49	0.92
2:E:282:GLN:H	2:E:282:GLN:HE21	1.16	0.91
2:E:257:ASN:HD21	2:E:259:PHE:HB3	1.35	0.91
4:H:85:ASN:HD21	4:H:91:GLN:HE22	1.13	0.90
2:D:282:GLN:H	2:D:282:GLN:HE21	0.91	0.88
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.87
2:D:282:GLN:H	2:D:282:GLN:NE2	1.71	0.86
2:F:282:GLN:H	2:F:282:GLN:NE2	1.77	0.81
4:H:105:LEU:HD22	4:H:109:LYS:HE3	1.63	0.81
1:B:47:VAL:HG12	1:B:90:ARG:HG2	1.62	0.81
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.63	0.81
3:G:89:MET:HB3	3:G:116:LEU:HD22	1.63	0.80
2:E:388:ILE:HG12	2:E:396:LEU:HD11	1.62	0.80
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.65	0.79
2:D:275:ILE:HD13	3:G:272:LEU:HD12	1.64	0.79
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.65	0.79
3:G:137:THR:HG21	5:I:39:GLY:H	1.48	0.78
2:D:282:GLN:N	2:D:282:GLN:HE21	1.76	0.77
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:117:HIS:ND1	3:G:118:ARG:N	2.34	0.76
2:D:10:THR:HG21	2:D:74:LYS:HE3	1.68	0.75
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.68	0.75
4:H:138:ASN:HA	4:H:141:LEU:HD12	1.68	0.74
3:G:121:SER:C	3:G:123:GLN:H	1.91	0.74
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.70	0.74
2:F:223:ASN:H	2:F:223:ASN:HD22	1.36	0.73
4:H:34:ARG:HH22	4:H:70:GLY:HA2	1.52	0.73
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.70	0.73
4:H:85:ASN:HD21	4:H:91:GLN:NE2	1.87	0.72
2:F:89:GLU:HB2	2:F:110:THR:HG22	1.71	0.72
1:C:183:ILE:HD12	1:C:201:CYS:HB3	1.69	0.72
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.71	0.72
3:G:57:ILE:CG2	3:G:184:ILE:HD12	2.19	0.72
1:B:406:PHE:CE1	1:B:410:LEU:HB2	2.25	0.72
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.72	0.72
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.71	0.71
2:D:89:GLU:HG3	2:D:110:THR:HA	1.71	0.71
2:E:390:ILE:O	2:E:391:LEU:HB2	1.90	0.71
4:H:133:ILE:HD11	5:I:4:TRP:HB3	1.73	0.71
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.72	0.70
1:B:102:GLU:HG3	1:B:123:SER:HA	1.74	0.69
1:B:343:ILE:HD12	1:B:349:GLN:HG2	1.75	0.69
1:B:246:ALA:HB3	1:B:247:PRO:HD3	1.74	0.68
2:E:170:ILE:HD13	2:E:215:VAL:HG11	1.75	0.67
3:G:137:THR:HG22	3:G:139:GLY:H	1.60	0.67
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.77	0.67
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.75	0.67
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.76	0.67
1:B:289:PRO:HG2	3:G:263:ILE:HD12	1.76	0.67
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.67
1:A:141:SER:O	1:A:143:ARG:HD3	1.95	0.67
1:B:30:ARG:NH1	1:B:32:LEU:HD23	2.10	0.67
2:E:282:GLN:H	2:E:282:GLN:NE2	1.92	0.66
2:F:444:ILE:HD11	2:F:463:ILE:HD11	1.78	0.66
2:E:408:ARG:O	2:E:412:ARG:HG2	1.94	0.66
2:F:410:ILE:HG13	2:F:444:ILE:HG21	1.78	0.66
2:E:9:THR:HG21	2:E:27:GLU:HG3	1.78	0.66
2:F:208:LEU:O	2:F:209:LYS:HE2	1.96	0.65
5:I:35:MET:C	5:I:37:THR:H	1.99	0.65
2:E:185:GLY:HA3	2:E:188:GLU:HG2	1.79	0.65
1:C:338:ILE:HB	1:C:339:PRO:HD3	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:440:GLY:O	2:F:444:ILE:HD13	1.97	0.65
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.62	0.64
2:F:471:ASP:C	2:F:473:LEU:H	2.01	0.64
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.79	0.64
3:G:115:ILE:C	3:G:117:HIS:H	2.01	0.64
4:H:54:THR:N	4:H:84:VAL:HG23	2.13	0.64
1:C:211:SER:HB3	2:F:126:MET:CE	2.28	0.63
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.63
1:B:168:ILE:HD11	1:B:329:THR:CG2	2.28	0.63
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.80	0.63
2:F:172:ASN:ND2	2:F:431:LEU:HD11	2.14	0.63
3:G:141:ALA:HB1	3:G:213:ILE:HG23	1.81	0.63
2:F:63:MET:CE	2:F:228:ALA:HA	2.29	0.63
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.79	0.63
2:D:139:VAL:HA	12:D:2048:HOH:O	1.99	0.63
1:B:410:LEU:HD21	1:B:414:THR:HB	1.80	0.63
3:G:61:GLU:OE1	3:G:101:LYS:HG2	1.99	0.62
2:D:258:ILE:HD11	2:D:292:MET:SD	2.39	0.62
1:C:52:MET:HE2	1:C:52:MET:HA	1.80	0.62
4:H:65:VAL:C	4:H:72:THR:HG23	2.19	0.62
4:H:54:THR:H	4:H:84:VAL:HG23	1.65	0.62
2:D:101:PRO:HB3	2:D:108:ILE:HD11	1.81	0.62
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.82	0.61
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.30	0.61
1:B:80:LYS:HD2	2:E:33:LEU:HD12	1.82	0.61
1:C:91:THR:HG23	1:C:93:ALA:H	1.65	0.61
3:G:178:ILE:C	3:G:180:SER:H	2.04	0.61
2:D:321:ALA:HB3	2:D:322:PRO:HD3	1.83	0.61
1:B:30:ARG:O	1:B:31:VAL:HB	2.01	0.61
2:D:143:LEU:HG	12:D:2048:HOH:O	2.00	0.61
2:F:63:MET:HE3	2:F:228:ALA:HA	1.83	0.60
2:D:136:GLY:HA3	2:D:431:LEU:CD1	2.32	0.60
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.82	0.60
1:A:183:ILE:HD12	1:A:201:CYS:HB3	1.83	0.60
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.84	0.60
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.83	0.60
1:A:362:ARG:HA	1:A:363:PRO:C	2.21	0.60
2:D:292:MET:HE2	2:D:293:GLN:HG2	1.83	0.60
2:D:393:MET:HG3	2:D:396:LEU:HD12	1.84	0.60
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.84	0.59
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.84	0.59
2:E:358:MET:HE2	2:E:368:TYR:HD1	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:20:ASP:HB3	1:B:22:SER:H	1.67	0.59
1:B:442:VAL:HG21	1:B:489:ILE:HD11	1.84	0.59
3:G:57:ILE:CG2	3:G:184:ILE:CD1	2.81	0.59
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.85	0.59
1:B:440:GLU:HB3	1:B:469:LEU:HD11	1.84	0.59
2:F:419:GLN:NE2	2:F:431:LEU:HD13	2.17	0.59
1:C:91:THR:CG2	1:C:93:ALA:H	2.16	0.59
3:G:207:TYR:HA	5:I:12:ILE:HD11	1.84	0.59
1:C:381:ARG:H	1:C:381:ARG:HD2	1.68	0.59
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.83	0.58
3:G:156:ASP:HA	3:G:181:LEU:HD13	1.85	0.58
2:E:390:ILE:CG2	3:G:29:ALA:HB2	2.33	0.58
1:A:151:LYS:HD3	1:A:436:MET:SD	2.43	0.58
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.84	0.58
2:D:419:GLN:HA	2:D:429:GLY:HA3	1.85	0.58
2:E:404:VAL:O	2:E:408:ARG:HG3	2.03	0.58
3:G:87:LYS:O	3:G:90:LYS:HG2	2.04	0.58
4:H:64:VAL:HG13	4:H:72:THR:HG21	1.85	0.58
1:A:44:LEU:O	1:A:47:VAL:HG22	2.04	0.58
1:A:383:MET:HE2	1:A:387:ALA:HB2	1.85	0.58
3:G:180:SER:O	3:G:205:GLN:HG3	2.04	0.58
1:B:362:ARG:HA	1:B:363:PRO:C	2.23	0.57
5:I:5:ARG:C	5:I:7:ALA:H	2.06	0.57
2:D:199:GLU:CG	10:D:700:DCW:C7	2.63	0.57
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.33	0.57
2:F:419:GLN:HE21	2:F:431:LEU:HD13	1.67	0.57
4:H:96:GLU:OE2	5:I:23:ARG:NE	2.38	0.57
1:B:146:MET:HE1	1:B:186:GLN:NE2	2.20	0.57
3:G:57:ILE:HG23	3:G:184:ILE:CD1	2.35	0.57
3:G:164:ARG:NH2	3:G:166:ARG:HD3	2.20	0.57
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.70	0.57
2:F:32:ILE:HD12	2:F:51:GLN:HA	1.86	0.56
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.56
1:A:96:ASP:OD1	1:A:126:ARG:NH1	2.38	0.56
1:A:499:GLU:HG2	1:A:500:ILE:N	2.20	0.56
2:E:339:ILE:HD12	2:E:349:ASP:HA	1.86	0.56
3:G:57:ILE:HG22	3:G:184:ILE:HD12	1.87	0.56
4:H:65:VAL:O	4:H:72:THR:HG23	2.05	0.56
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.87	0.56
1:A:211:SER:HB3	2:D:126:MET:CE	2.35	0.56
1:B:99:VAL:HG22	1:B:253:MET:HA	1.88	0.56
1:C:246:ALA:HB3	1:C:247:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:137:THR:HG21	5:I:39:GLY:N	2.19	0.56
1:B:295:PRO:O	1:B:298:VAL:HG22	2.06	0.56
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.86	0.56
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.87	0.56
2:D:188:GLU:H	2:D:221:GLN:NE2	2.04	0.56
3:G:184:ILE:C	3:G:186:SER:H	2.08	0.55
1:B:171:ARG:HB2	1:B:171:ARG:NH1	2.21	0.55
1:A:49:ALA:O	1:A:50:GLU:HB2	2.07	0.55
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.71	0.55
1:C:49:ALA:O	1:C:50:GLU:HB2	2.05	0.55
2:F:433:PRO:HD2	2:F:436:GLU:HG3	1.88	0.55
3:G:160:ILE:CG2	3:G:176:LYS:HB2	2.36	0.55
2:F:470:ALA:HA	2:F:473:LEU:HD12	1.87	0.55
2:E:223:ASN:H	2:E:223:ASN:HD22	1.55	0.55
3:G:181:LEU:HG	3:G:183:THR:HB	1.89	0.55
2:E:89:GLU:HG2	2:E:110:THR:CG2	2.35	0.55
3:G:207:TYR:HA	5:I:12:ILE:CD1	2.37	0.55
1:A:151:LYS:HE3	1:A:427:LEU:O	2.06	0.55
1:B:168:ILE:HD13	1:B:169:GLY:N	2.21	0.55
12:G:2006:HOH:O	5:I:41:THR:HG21	2.06	0.55
2:F:130:GLN:HB3	2:F:357:ILE:CD1	2.37	0.55
3:G:121:SER:C	3:G:123:GLN:N	2.60	0.55
1:A:211:SER:HB3	2:D:126:MET:HE2	1.87	0.55
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.88	0.55
1:B:142:VAL:HG13	12:B:2038:HOH:O	2.06	0.55
2:F:225:PRO:HG3	12:F:2025:HOH:O	2.05	0.55
1:C:362:ARG:HA	1:C:363:PRO:C	2.26	0.55
3:G:117:HIS:ND1	3:G:118:ARG:HA	2.22	0.54
3:G:117:HIS:CE1	3:G:121:SER:HB2	2.42	0.54
3:G:181:LEU:HB3	3:G:184:ILE:HG22	1.89	0.54
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.39	0.54
2:F:282:GLN:HE21	2:F:282:GLN:N	1.85	0.54
1:C:488:LYS:HG2	1:C:489:ILE:N	2.23	0.54
3:G:181:LEU:O	3:G:184:ILE:HG22	2.08	0.54
3:G:144:ILE:HD13	3:G:213:ILE:HD11	1.90	0.54
2:F:245:ASP:C	2:F:247:GLU:H	2.11	0.54
2:F:471:ASP:C	2:F:473:LEU:N	2.61	0.54
3:G:164:ARG:HD3	3:G:174:GLU:OE2	2.07	0.54
1:C:99:VAL:HG22	1:C:253:MET:HA	1.90	0.54
2:F:87:GLY:HA2	2:F:242:TYR:CE1	2.43	0.54
1:C:215:GLN:HE22	2:F:128:VAL:HA	1.73	0.54
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:410:LEU:HG	1:B:411:ASP:H	1.72	0.54
1:C:52:MET:HB3	1:C:91:THR:HG21	1.90	0.54
1:B:416:GLN:O	1:B:419:SER:HB3	2.07	0.54
2:F:360:PRO:HD3	2:F:368:TYR:CD1	2.43	0.54
4:H:22:SER:HB2	4:H:23:PRO:HD2	1.89	0.54
3:G:71:VAL:HG13	3:G:108:VAL:HG22	1.88	0.54
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
2:D:139:VAL:HB	12:D:2047:HOH:O	2.06	0.53
2:D:142:LEU:HD23	12:D:2048:HOH:O	2.08	0.53
2:D:63:MET:HE3	2:D:228:ALA:HA	1.89	0.53
1:B:168:ILE:HD11	1:B:329:THR:HG21	1.89	0.53
1:C:441:GLN:O	1:C:445:ILE:HG12	2.08	0.53
5:I:28:THR:O	5:I:29:GLU:HB2	2.08	0.53
1:C:211:SER:HB3	2:F:126:MET:HE2	1.90	0.53
1:C:211:SER:HB3	2:F:126:MET:HE1	1.90	0.53
1:B:406:PHE:CZ	1:B:410:LEU:HD22	2.43	0.53
1:B:482:LYS:NZ	1:B:496:LYS:NZ	2.56	0.53
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.38	0.53
1:C:347:ASP:C	1:C:373:ARG:HG3	2.28	0.53
2:E:408:ARG:HH21	2:E:412:ARG:HH22	1.56	0.53
2:F:172:ASN:HD21	2:F:431:LEU:HD11	1.73	0.53
3:G:137:THR:HG22	3:G:138:PHE:N	2.24	0.53
1:B:168:ILE:HD11	1:B:329:THR:HG23	1.91	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53
2:D:63:MET:CE	2:D:97:VAL:HG11	2.39	0.52
2:D:310:ILE:HD13	2:D:325:THR:HG21	1.91	0.52
1:A:381:ARG:HD2	1:A:487:GLY:O	2.08	0.52
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.25	0.52
5:I:5:ARG:O	5:I:6:GLN:HB3	2.10	0.52
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.91	0.52
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.52
4:H:127:THR:O	4:H:131:ILE:HG12	2.10	0.52
2:D:63:MET:CE	2:D:228:ALA:HA	2.39	0.52
2:F:63:MET:CE	2:F:97:VAL:HG11	2.40	0.52
2:E:51:GLN:HE21	2:E:272:LEU:HD22	1.74	0.52
4:H:40:THR:HG23	4:H:42:THR:H	1.75	0.52
1:C:114:ALA:HB2	1:C:121:ILE:HD12	1.91	0.52
2:F:292:MET:CE	2:F:296:ILE:HD11	2.40	0.52
1:C:179:ALA:O	1:C:183:ILE:HG12	2.09	0.52
2:E:257:ASN:ND2	2:E:259:PHE:H	2.08	0.52
1:A:362:ARG:HH22	2:D:372:ARG:HD3	1.74	0.52
2:D:420:VAL:HG13	10:D:700:DCW:H8	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:LEU:HG	1:B:65:ASN:ND2	2.24	0.52
3:G:117:HIS:O	3:G:120:HIS:N	2.35	0.52
3:G:117:HIS:ND1	3:G:118:ARG:CA	2.73	0.52
2:D:63:MET:HE1	2:D:97:VAL:HG11	1.91	0.52
3:G:19:ILE:HG22	3:G:23:MET:CE	2.40	0.52
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.52
4:H:34:ARG:HG2	4:H:66:HIS:O	2.10	0.51
1:B:24:ASP:O	1:B:28:THR:HB	2.11	0.51
1:C:419:SER:O	1:C:423:ARG:HG2	2.10	0.51
1:B:469:LEU:O	1:B:473:ILE:HG12	2.10	0.51
1:A:336:ALA:HB3	1:A:339:PRO:HG2	1.92	0.51
1:C:74:VAL:HG13	1:C:241:PRO:HB3	1.93	0.51
2:F:337:ARG:O	2:F:341:GLU:HG3	2.10	0.51
2:F:440:GLY:HA2	2:F:463:ILE:HG13	1.91	0.51
2:E:358:MET:HE2	2:E:368:TYR:CD1	2.46	0.51
2:E:80:ALA:HB1	2:E:81:PRO:CD	2.40	0.51
2:D:397:SER:O	2:D:401:LYS:HD2	2.10	0.51
3:G:49:LEU:HD21	3:G:212:ILE:CD1	2.41	0.51
2:D:97:VAL:HG13	2:D:232:VAL:HG13	1.93	0.51
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.45	0.51
1:C:185:ASN:OD1	1:C:435:PRO:HB2	2.11	0.51
2:D:139:VAL:HG22	2:D:414:LEU:HD22	1.92	0.51
1:C:52:MET:HE3	1:C:76:PHE:HE2	1.76	0.51
4:H:83:THR:HB	4:H:91:GLN:HE21	1.75	0.51
1:C:211:SER:O	1:C:215:GLN:HG2	2.11	0.51
1:B:26:GLU:HA	1:B:45:ARG:HB2	1.93	0.51
1:C:418:LEU:O	1:C:422:VAL:HG23	2.10	0.50
1:B:457:GLU:OE1	1:B:460:LYS:HG3	2.10	0.50
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.92	0.50
4:H:18:PHE:CZ	4:H:20:PHE:HB2	2.46	0.50
2:D:95:MET:HG3	12:D:2063:HOH:O	2.11	0.50
2:F:63:MET:HE1	2:F:97:VAL:HG11	1.92	0.50
2:D:136:GLY:HA3	2:D:431:LEU:HD12	1.92	0.50
2:D:167:MET:HG3	10:D:700:DCW:H131	1.94	0.50
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.44	0.50
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.50
1:A:338:ILE:N	1:A:339:PRO:CD	2.75	0.50
2:F:96:ASN:ND2	2:F:100:GLU:H	2.09	0.50
1:B:156:LEU:HD22	1:B:391:LYS:HD3	1.94	0.50
2:E:408:ARG:HH21	2:E:412:ARG:NH2	2.10	0.50
2:F:246:GLN:O	2:F:247:GLU:HG3	2.12	0.49
4:H:35:GLN:HB3	4:H:66:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.94	0.49
2:F:345:TYR:HA	2:F:346:PRO:C	2.33	0.49
1:B:30:ARG:HH11	1:B:32:LEU:HD23	1.76	0.49
1:B:171:ARG:HB2	1:B:171:ARG:HH11	1.76	0.49
4:H:138:ASN:O	4:H:141:LEU:HB2	2.12	0.49
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.42	0.49
1:A:270:ASP:HB2	1:A:326:VAL:O	2.13	0.49
1:C:36:ASP:HB3	1:C:284:LEU:HD13	1.93	0.49
1:A:496:LYS:HA	1:A:499:GLU:CD	2.32	0.49
3:G:71:VAL:HG13	3:G:108:VAL:CG2	2.43	0.49
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.93	0.49
2:D:399:GLU:O	2:D:403:THR:HG23	2.12	0.49
2:D:15:ALA:HB3	2:D:22:ASP:HB2	1.94	0.49
1:A:205:ALA:C	1:A:206:ILE:HG13	2.33	0.49
3:G:179:PHE:C	3:G:181:LEU:N	2.66	0.49
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.95	0.49
1:A:395:ALA:HA	1:A:398:ARG:NH1	2.27	0.49
4:H:105:LEU:CD2	4:H:109:LYS:HE3	2.41	0.49
2:F:292:MET:HE2	2:F:296:ILE:HD11	1.94	0.49
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.46	0.49
2:E:258:ILE:O	2:E:258:ILE:HD13	2.13	0.49
1:B:339:PRO:O	1:B:343:ILE:HG12	2.13	0.49
1:A:496:LYS:HA	1:A:499:GLU:OE2	2.13	0.49
1:A:496:LYS:HD2	1:A:499:GLU:OE2	2.13	0.49
4:H:41:GLN:HG2	4:H:57:VAL:HG12	1.94	0.49
1:B:388:GLY:O	1:B:392:LEU:HD23	2.13	0.49
2:D:10:THR:CG2	2:D:74:LYS:HE3	2.39	0.48
3:G:203:ASN:CB	4:H:57:VAL:HG21	2.42	0.48
2:E:408:ARG:O	2:E:411:GLN:HG2	2.13	0.48
2:F:266:SER:HB2	2:F:282:GLN:HE22	1.79	0.48
3:G:156:ASP:O	3:G:181:LEU:HB2	2.13	0.48
4:H:34:ARG:HH22	4:H:70:GLY:CA	2.24	0.48
2:D:136:GLY:HA3	2:D:431:LEU:HD11	1.94	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.76	0.48
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.95	0.48
1:A:195:GLU:HA	1:A:198:LYS:HG3	1.94	0.48
1:C:180:ILE:HD11	1:C:216:LEU:CD2	2.44	0.48
4:H:105:LEU:HG	4:H:145:LEU:HB3	1.94	0.48
1:C:183:ILE:HD11	1:C:267:ILE:CD1	2.43	0.48
1:B:468:PHE:CZ	1:B:501:VAL:HG12	2.48	0.48
2:E:48:GLU:HB3	2:E:61:ILE:CD1	2.44	0.48
2:E:48:GLU:O	2:E:61:ILE:HD13	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:197:ASP:O	3:G:200:VAL:HG12	2.13	0.48
2:E:359:ASP:OD2	2:E:361:ASN:HB2	2.13	0.48
1:B:78:ASN:ND2	2:E:119:GLU:OE2	2.46	0.48
3:G:160:ILE:HG22	3:G:176:LYS:HB2	1.95	0.48
1:C:99:VAL:CG2	1:C:253:MET:HA	2.43	0.48
1:B:130:GLY:HA2	9:B:701:GOL:H11	1.96	0.48
2:D:420:VAL:HG22	10:D:700:DCW:H31C	1.96	0.48
2:D:139:VAL:HG21	12:D:2115:HOH:O	2.14	0.48
2:E:339:ILE:CD1	2:E:349:ASP:HA	2.44	0.48
1:C:105:GLY:HA2	1:C:226:MET:O	2.12	0.48
1:B:211:SER:HB3	2:E:126:MET:HE1	1.96	0.48
2:E:282:GLN:N	2:E:282:GLN:HE21	1.98	0.48
2:E:89:GLU:HG3	2:E:109:LYS:O	2.14	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.44	0.48
2:D:276:PRO:HG3	3:G:268:GLY:HA3	1.94	0.48
2:D:237:LEU:HD11	2:D:295:ARG:NE	2.29	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.96	0.48
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.48	0.48
2:D:9:THR:HG21	2:D:28:GLY:O	2.14	0.48
3:G:179:PHE:HB3	3:G:184:ILE:HG21	1.96	0.47
1:C:183:ILE:HD11	1:C:267:ILE:HD12	1.95	0.47
2:F:360:PRO:HD3	2:F:368:TYR:CE1	2.49	0.47
2:F:391:LEU:HD13	2:F:395:GLU:HG2	1.95	0.47
2:F:400:ASP:O	2:F:404:VAL:HG23	2.14	0.47
3:G:89:MET:CB	3:G:116:LEU:HD22	2.38	0.47
5:I:37:THR:HG22	5:I:38:SER:H	1.80	0.47
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.95	0.47
4:H:57:VAL:HG13	5:I:11:TYR:CZ	2.50	0.47
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.47
3:G:117:HIS:ND1	3:G:117:HIS:C	2.67	0.47
1:B:292:GLU:O	1:B:293:ALA:HB3	2.14	0.47
1:B:49:ALA:O	1:B:50:GLU:HB2	2.15	0.47
1:B:185:ASN:O	1:B:188:ARG:HG2	2.15	0.47
2:D:390:ILE:HD12	3:G:16:ILE:CD1	2.44	0.47
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.50	0.47
3:G:129:LYS:HG2	3:G:130:GLU:OE1	2.14	0.47
3:G:179:PHE:O	3:G:181:LEU:N	2.48	0.47
1:B:338:ILE:N	1:B:339:PRO:CD	2.77	0.47
1:C:338:ILE:N	1:C:339:PRO:CD	2.77	0.47
2:E:367:HIS:ND1	2:E:438:ILE:HD11	2.30	0.47
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:87:GLY:HA2	2:D:242:TYR:CE1	2.50	0.47
3:G:125:LEU:HD11	3:G:151:SER:HB2	1.96	0.47
2:F:196:LEU:HD11	2:F:200:MET:CE	2.45	0.47
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.45	0.47
1:B:457:GLU:O	1:B:460:LYS:N	2.42	0.47
2:F:394:ASP:HB2	12:F:2143:HOH:O	2.14	0.47
2:D:139:VAL:HG23	12:D:2133:HOH:O	2.15	0.47
2:D:224:GLU:HB3	2:D:225:PRO:HD2	1.97	0.47
4:H:47:ILE:H	4:H:47:ILE:HD12	1.79	0.47
2:E:179:GLY:HA3	2:E:250:ASP:O	2.14	0.47
2:D:369:ASP:OD1	2:D:372:ARG:NH2	2.47	0.47
2:E:345:TYR:HA	2:E:346:PRO:C	2.35	0.47
3:G:207:TYR:CZ	4:H:80:GLY:HA2	2.50	0.46
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.96	0.46
2:D:84:ILE:HB	2:D:85:PRO:HD2	1.96	0.46
1:A:34:ILE:HD12	1:A:38:ILE:O	2.16	0.46
2:F:188:GLU:O	2:F:222:MET:HG2	2.15	0.46
1:C:201:CYS:O	1:C:229:THR:HA	2.15	0.46
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.44	0.46
3:G:144:ILE:HG21	3:G:213:ILE:HD13	1.97	0.46
2:E:406:ARG:O	2:E:410:ILE:HG12	2.16	0.46
2:F:366:GLU:O	2:F:370:VAL:HG23	2.16	0.46
1:C:188:ARG:NH2	1:C:437:ALA:N	2.64	0.46
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.98	0.46
2:D:348:VAL:O	2:D:350:PRO:HD3	2.15	0.46
1:A:497:LEU:O	1:A:501:VAL:HG12	2.15	0.46
1:C:288:PRO:HG2	2:D:270:ALA:HB1	1.98	0.46
2:F:443:GLN:HE21	2:F:449:TYR:HE2	1.62	0.46
1:A:299:PHE:CZ	1:A:345:ILE:HD11	2.50	0.46
1:A:32:LEU:HD21	1:A:42:HIS:HB2	1.96	0.46
1:B:357:PHE:C	1:B:359:LYS:H	2.19	0.46
1:B:380:THR:HG22	1:B:383:MET:H	1.81	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.51	0.46
4:H:70:GLY:O	4:H:71:THR:C	2.53	0.46
2:E:471:ASP:O	2:E:472:LYS:C	2.54	0.46
2:E:380:ASP:O	2:E:384:LEU:HG	2.15	0.46
4:H:99:THR:O	4:H:102:MET:HG2	2.15	0.46
1:B:409:ASP:HB3	3:G:169:ILE:HD11	1.98	0.46
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.45	0.46
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.46
1:A:392:LEU:HG	1:A:396:GLN:NE2	2.30	0.46
2:F:225:PRO:HB2	12:F:2020:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:16:VAL:O	2:F:17:ILE:HD13	2.16	0.46
2:E:393:MET:C	2:E:395:GLU:H	2.19	0.46
1:B:354:THR:HG23	1:B:358:TYR:CE1	2.51	0.46
4:H:35:GLN:HB3	4:H:66:HIS:CD2	2.50	0.45
2:D:97:VAL:HG22	12:D:2064:HOH:O	2.16	0.45
2:F:63:MET:HE1	2:F:228:ALA:HA	1.98	0.45
2:F:405:SER:O	2:F:409:LYS:HG3	2.16	0.45
2:E:163:THR:O	2:E:167:MET:HG3	2.16	0.45
2:E:27:GLU:CD	2:E:27:GLU:H	2.19	0.45
5:I:35:MET:C	5:I:37:THR:N	2.68	0.45
3:G:206:GLU:O	5:I:12:ILE:HD11	2.17	0.45
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.98	0.45
1:B:403:PHE:O	1:B:404:ALA:C	2.53	0.45
2:E:181:SER:HB2	2:E:215:VAL:CG1	2.33	0.45
2:D:279:VAL:O	2:D:279:VAL:HG12	2.16	0.45
1:B:87:ILE:HD12	1:B:87:ILE:H	1.82	0.45
1:B:399:GLU:C	1:B:400:VAL:HG23	2.36	0.45
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.45
1:A:481:GLY:HA2	1:A:484:ARG:NH1	2.31	0.45
1:B:410:LEU:HB3	1:B:415:GLN:CG	2.46	0.45
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.45
4:H:112:LEU:HD21	4:H:135:ILE:HG23	1.99	0.45
3:G:51:LEU:HD13	4:H:55:LEU:HD21	1.97	0.45
1:B:289:PRO:CG	3:G:263:ILE:HD12	2.46	0.45
3:G:86:ALA:HA	3:G:89:MET:HE2	1.99	0.45
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.45
1:A:114:ALA:HB2	1:A:121:ILE:CD1	2.47	0.45
1:B:47:VAL:CG1	1:B:90:ARG:HG2	2.41	0.45
2:E:400:ASP:O	2:E:404:VAL:HG23	2.17	0.45
1:C:30:ARG:HA	1:C:86:ASP:O	2.15	0.45
2:E:135:THR:OG1	2:E:137:ILE:HB	2.17	0.45
3:G:115:ILE:C	3:G:117:HIS:N	2.68	0.45
1:B:295:PRO:HB2	1:B:297:ASP:OD1	2.16	0.45
2:F:96:ASN:HD21	2:F:100:GLU:H	1.64	0.45
3:G:178:ILE:C	3:G:180:SER:N	2.69	0.44
2:E:228:ALA:O	2:E:232:VAL:HG22	2.16	0.44
1:A:362:ARG:HH22	2:D:372:ARG:CG	2.31	0.44
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.44
3:G:105:ILE:HG22	3:G:106:ILE:N	2.32	0.44
3:G:117:HIS:CE1	3:G:118:ARG:NE	2.86	0.44
2:F:223:ASN:H	2:F:223:ASN:ND2	2.10	0.44
4:H:55:LEU:O	4:H:56:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:333:ASP:OD2	3:G:252:ARG:HD3	2.17	0.44
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.99	0.44
1:B:286:ARG:NE	12:B:2079:HOH:O	2.48	0.44
2:E:61:ILE:H	2:E:61:ILE:HD13	1.83	0.44
1:C:411:ASP:OD2	1:C:413:ALA:HB3	2.18	0.44
2:E:422:GLU:HG2	2:E:427:HIS:O	2.17	0.44
2:D:145:PRO:HD2	2:D:358:MET:HG2	1.98	0.44
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.52	0.44
3:G:84:SER:HB3	3:G:173:THR:OG1	2.17	0.44
2:E:397:SER:O	2:E:401:LYS:HG3	2.18	0.44
2:E:381:TYR:CE1	2:E:404:VAL:HG13	2.52	0.44
1:A:183:ILE:HD11	1:A:267:ILE:HD12	2.00	0.44
2:F:432:VAL:HA	2:F:433:PRO:HD3	1.83	0.44
2:E:223:ASN:N	2:E:223:ASN:HD22	2.15	0.44
1:A:338:ILE:N	1:A:339:PRO:HD2	2.33	0.44
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.99	0.44
4:H:33:VAL:HG11	4:H:65:VAL:HG13	1.99	0.44
1:A:383:MET:CE	1:A:386:VAL:HG23	2.47	0.44
1:B:297:ASP:HB3	2:F:267:GLU:HG2	1.99	0.44
2:E:183:PHE:HB3	2:E:217:LEU:HD23	2.00	0.44
1:B:359:LYS:HD2	1:B:361:ILE:CD1	2.48	0.44
3:G:128:PHE:HB3	5:I:42:ILE:CD1	2.48	0.44
1:C:23:VAL:O	1:C:23:VAL:HG12	2.18	0.44
1:A:165:GLU:O	1:A:325:PRO:HD2	2.17	0.44
3:G:113:ARG:O	3:G:117:HIS:HB2	2.18	0.44
2:D:97:VAL:HG13	2:D:232:VAL:CG1	2.47	0.44
1:C:33:SER:HB2	2:F:52:HIS:O	2.17	0.44
2:D:142:LEU:HB3	12:D:2048:HOH:O	2.17	0.44
1:B:482:LYS:NZ	1:B:496:LYS:HZ2	2.15	0.44
1:A:345:ILE:HD13	2:E:222:MET:SD	2.58	0.44
1:B:209:LYS:HD2	2:E:328:HIS:HA	2.00	0.44
1:C:381:ARG:N	1:C:381:ARG:HD2	2.32	0.43
1:C:362:ARG:HD3	6:C:600:ATP:C2	2.53	0.43
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.99	0.43
1:C:444:VAL:HG12	1:C:469:LEU:HD13	2.00	0.43
2:D:32:ILE:O	2:D:33:LEU:HB2	2.18	0.43
1:C:404:ALA:C	1:C:406:PHE:H	2.21	0.43
1:B:410:LEU:HG	1:B:414:THR:OG1	2.18	0.43
2:E:257:ASN:HD22	2:E:260:ARG:H	1.65	0.43
2:E:63:MET:HE3	2:E:97:VAL:HG21	1.99	0.43
1:A:422:VAL:O	1:A:426:GLU:HG2	2.18	0.43
1:B:168:ILE:C	1:B:168:ILE:HD13	2.38	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:ALA:N	1:A:241:PRO:CD	2.81	0.43
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.48	0.43
2:D:237:LEU:HD11	2:D:295:ARG:CZ	2.48	0.43
1:A:20:ASP:O	1:A:22:SER:N	2.51	0.43
2:F:223:ASN:N	2:F:223:ASN:HD22	2.07	0.43
2:E:358:MET:CE	2:E:368:TYR:HA	2.49	0.43
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
1:B:158:PRO:O	1:B:375:GLY:HA3	2.19	0.43
2:E:415:SER:HB2	2:E:459:MET:H	1.84	0.43
1:C:62:MET:HG2	1:C:64:LEU:HD13	2.01	0.43
2:D:139:VAL:HG22	2:D:414:LEU:HB3	2.00	0.43
2:F:245:ASP:O	2:F:247:GLU:N	2.50	0.43
1:A:440:GLU:O	1:A:444:VAL:HG13	2.19	0.43
2:E:419:GLN:N	2:E:429:GLY:HA3	2.33	0.43
1:B:406:PHE:CZ	1:B:410:LEU:HD13	2.53	0.43
2:D:89:GLU:HB2	2:D:110:THR:HG23	2.01	0.43
2:F:348:VAL:O	2:F:350:PRO:HD3	2.18	0.43
2:E:170:ILE:CD1	2:E:215:VAL:HG11	2.46	0.43
4:H:41:GLN:CG	4:H:57:VAL:HG12	2.48	0.43
1:B:508:PHE:CE2	1:B:510:ALA:HA	2.53	0.43
1:B:148:THR:HA	1:B:182:THR:HG23	2.01	0.43
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.99	0.43
2:D:188:GLU:O	2:D:221:GLN:HB3	2.18	0.43
1:A:487:GLY:O	1:A:488:LYS:HB3	2.19	0.43
4:H:79:SER:O	4:H:94:ALA:HA	2.18	0.43
1:C:410:LEU:O	1:C:415:GLN:NE2	2.51	0.43
3:G:86:ALA:O	3:G:116:LEU:HD13	2.18	0.43
4:H:35:GLN:HG2	4:H:36:VAL:N	2.34	0.43
2:F:51:GLN:HG2	2:F:59:ARG:HB3	2.00	0.43
1:C:151:LYS:HA	1:C:441:GLN:OE1	2.17	0.43
1:A:446:TYR:O	1:A:449:VAL:HG12	2.19	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.43
4:H:131:ILE:HG23	4:H:134:ARG:HH21	1.84	0.43
4:H:20:PHE:CD1	4:H:92:LEU:HD23	2.54	0.43
1:C:240:ALA:N	1:C:241:PRO:CD	2.82	0.42
2:E:48:GLU:HB3	2:E:61:ILE:HD11	1.99	0.42
1:B:286:ARG:HG2	2:E:275:ILE:CD1	2.49	0.42
1:A:157:VAL:N	1:A:158:PRO:CD	2.82	0.42
1:A:423:ARG:NH2	1:A:458:PRO:HD3	2.33	0.42
1:B:269:ASP:HA	1:B:270:ASP:HA	1.74	0.42
2:E:221:GLN:N	2:E:224:GLU:OE2	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:192:ILE:HG22	4:H:53:PRO:HG2	2.00	0.42
3:G:180:SER:O	3:G:182:ASP:N	2.52	0.42
2:E:387:ILE:O	2:E:391:LEU:HB3	2.18	0.42
1:A:49:ALA:O	1:A:50:GLU:CB	2.66	0.42
1:B:156:LEU:HD13	1:B:367:VAL:HG11	2.00	0.42
1:C:189:PHE:HB3	1:C:197:LYS:HB3	2.01	0.42
2:E:335:LEU:HA	2:E:347:ALA:O	2.19	0.42
4:H:39:PRO:HG3	4:H:62:LEU:N	2.34	0.42
2:F:228:ALA:O	2:F:232:VAL:HG22	2.19	0.42
1:A:183:ILE:HD12	1:A:201:CYS:SG	2.58	0.42
2:E:358:MET:HA	2:E:358:MET:HE3	2.01	0.42
1:B:157:VAL:N	1:B:158:PRO:CD	2.81	0.42
2:D:404:VAL:O	2:D:408:ARG:HG3	2.19	0.42
2:E:154:LEU:HD21	2:E:162:LYS:HG3	2.01	0.42
3:G:86:ALA:HA	3:G:89:MET:CE	2.49	0.42
3:G:87:LYS:HA	3:G:90:LYS:HE2	2.02	0.42
2:F:321:ALA:CB	2:F:322:PRO:CD	2.96	0.42
2:D:186:VAL:HG13	2:D:232:VAL:HG23	2.00	0.42
1:B:413:ALA:O	1:B:417:LEU:HG	2.20	0.42
1:A:102:GLU:HG2	1:A:122:GLY:O	2.19	0.42
3:G:180:SER:O	3:G:181:LEU:C	2.56	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.18	0.42
1:B:303:SER:HA	1:B:345:ILE:HD12	2.01	0.42
1:B:97:VAL:HB	1:B:98:PRO:CD	2.46	0.42
5:I:5:ARG:C	5:I:7:ALA:N	2.72	0.42
2:F:32:ILE:CD1	2:F:51:GLN:HA	2.50	0.42
1:B:171:ARG:HG2	12:B:2107:HOH:O	2.19	0.42
2:F:422:GLU:HG2	2:F:427:HIS:O	2.19	0.42
1:A:99:VAL:CG2	1:A:253:MET:HA	2.49	0.42
1:C:204:VAL:HG12	1:C:206:ILE:CD1	2.50	0.42
2:F:444:ILE:HD12	2:F:449:TYR:HD2	1.85	0.42
2:F:97:VAL:HG22	12:F:2073:HOH:O	2.18	0.42
1:A:362:ARG:HH22	2:D:372:ARG:CD	2.33	0.42
2:E:321:ALA:N	2:E:322:PRO:HD2	2.35	0.42
1:A:338:ILE:HB	1:A:339:PRO:HD3	2.02	0.42
2:F:416:GLN:HA	2:F:417:PRO:HD3	1.89	0.42
2:D:155:PHE:O	2:D:335:LEU:HB2	2.19	0.42
3:G:56:ASP:C	3:G:57:ILE:HG12	2.41	0.42
3:G:106:ILE:HG12	3:G:126:VAL:HG23	2.02	0.42
1:C:406:PHE:CE1	2:D:389:ALA:HA	2.54	0.42
1:B:390:MET:O	1:B:394:LEU:HB2	2.19	0.42
5:I:5:ARG:O	5:I:6:GLN:CB	2.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:ASP:HA	1:A:270:ASP:HA	1.77	0.42
2:D:242:TYR:CD2	2:D:246:GLN:HG3	2.55	0.42
1:C:171:ARG:NH1	12:C:2053:HOH:O	2.53	0.42
1:A:97:VAL:HB	1:A:98:PRO:HD2	2.02	0.42
1:A:183:ILE:HD12	1:A:201:CYS:CB	2.47	0.41
1:B:45:ARG:HD3	1:B:45:ARG:HA	1.88	0.41
1:A:48:GLN:HG2	2:E:70:VAL:HG22	2.02	0.41
1:B:404:ALA:O	1:B:406:PHE:CD1	2.74	0.41
4:H:34:ARG:NH2	4:H:70:GLY:HA2	2.28	0.41
3:G:203:ASN:HB3	4:H:57:VAL:HG21	2.02	0.41
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.55	0.41
3:G:184:ILE:C	3:G:186:SER:N	2.72	0.41
1:B:168:ILE:HD11	1:B:334:VAL:HG12	2.03	0.41
1:A:241:PRO:O	1:A:244:TYR:HB3	2.20	0.41
2:F:94:ILE:HG12	2:F:217:LEU:HD12	2.01	0.41
2:E:319:ASP:O	2:E:322:PRO:HD2	2.20	0.41
3:G:203:ASN:HB2	4:H:57:VAL:HG21	2.02	0.41
1:A:20:ASP:O	1:A:21:THR:C	2.59	0.41
2:F:314:ALA:O	2:F:315:ASP:HB2	2.21	0.41
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.41
1:C:194:ASP:OD2	1:C:197:LYS:HG3	2.20	0.41
1:B:406:PHE:HD1	1:B:407:GLY:N	2.18	0.41
4:H:62:LEU:CD1	4:H:144:ALA:HB2	2.34	0.41
2:F:471:ASP:O	2:F:473:LEU:N	2.54	0.41
1:C:180:ILE:HD11	1:C:216:LEU:HD21	2.01	0.41
1:A:62:MET:HE1	1:A:64:LEU:HD21	2.01	0.41
1:C:189:PHE:CD1	1:C:197:LYS:HD3	2.55	0.41
1:C:452:TYR:CD2	1:C:501:VAL:HG21	2.56	0.41
1:A:168:ILE:HD11	1:A:329:THR:CG2	2.51	0.41
1:B:404:ALA:O	1:B:405:GLN:C	2.59	0.41
3:G:120:HIS:HB3	3:G:123:GLN:HB2	2.03	0.41
2:E:63:MET:CE	2:E:228:ALA:HA	2.51	0.41
1:A:213:VAL:O	1:A:217:VAL:HG13	2.20	0.41
5:I:35:MET:O	5:I:37:THR:N	2.52	0.41
1:C:400:VAL:HG11	1:C:417:LEU:HD23	2.03	0.41
2:F:384:LEU:O	2:F:386:ASP:N	2.54	0.41
4:H:54:THR:O	4:H:55:LEU:HD23	2.20	0.41
1:B:473:ILE:O	1:B:477:GLN:HG2	2.21	0.41
1:C:362:ARG:NH1	12:C:2122:HOH:O	2.54	0.41
1:B:158:PRO:HG2	1:B:376:SER:HA	2.03	0.41
1:A:279:ARG:HG3	12:A:2097:HOH:O	2.20	0.41
2:E:95:MET:HG3	2:E:99:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:398:GLU:HA	2:F:401:LYS:HD2	2.02	0.41
2:D:274:ARG:O	3:G:272:LEU:HD11	2.21	0.41
2:F:357:ILE:CD1	2:F:362:ILE:HD13	2.51	0.41
1:B:168:ILE:CD1	1:B:334:VAL:HG12	2.50	0.41
1:C:304:ARG:HH11	1:C:304:ARG:HD3	1.71	0.41
12:A:2128:HOH:O	2:D:354:THR:HG22	2.20	0.41
1:B:410:LEU:HG	1:B:411:ASP:N	2.36	0.40
4:H:62:LEU:HD23	4:H:75:TYR:O	2.22	0.40
2:E:32:ILE:O	2:E:33:LEU:HB2	2.21	0.40
1:A:307:GLU:HG3	2:E:223:ASN:HB3	2.03	0.40
1:C:114:ALA:HB2	1:C:121:ILE:CD1	2.52	0.40
1:C:452:TYR:OH	1:C:498:LYS:HG3	2.21	0.40
1:C:144:GLU:HA	1:C:145:PRO:HD3	1.92	0.40
1:C:263:HIS:HD2	1:C:320:SER:OG	2.04	0.40
3:G:73:SER:O	3:G:111:LYS:HB2	2.21	0.40
2:D:382:LYS:HA	2:D:385:GLN:HE21	1.86	0.40
3:G:180:SER:O	3:G:205:GLN:NE2	2.50	0.40
1:B:185:ASN:OD1	1:B:435:PRO:HB2	2.21	0.40
2:D:246:GLN:O	2:D:247:GLU:HG3	2.21	0.40
1:B:268:TYR:O	1:B:270:ASP:HA	2.20	0.40
1:A:295:PRO:HD3	12:A:2097:HOH:O	2.21	0.40
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.40
3:G:184:ILE:O	3:G:184:ILE:HD13	2.22	0.40
3:G:51:LEU:HD23	3:G:52:TYR:CZ	2.57	0.40
1:A:398:ARG:NH2	12:A:2137:HOH:O	2.45	0.40
3:G:2:THR:C	3:G:4:LYS:N	2.75	0.40
1:C:237:SER:HB3	2:F:294:GLU:HG3	2.03	0.40
1:C:269:ASP:HA	1:C:270:ASP:HA	1.74	0.40
2:D:428:LEU:HD12	2:D:428:LEU:HA	1.97	0.40
1:A:138:PRO:HB3	1:A:316:PHE:CE1	2.55	0.40
4:H:78:SER:HB3	5:I:22:VAL:HG21	2.03	0.40
2:F:443:GLN:NE2	2:F:449:TYR:OH	2.54	0.40
4:H:40:THR:HG23	4:H:42:THR:N	2.36	0.40
1:C:48:GLN:HB2	1:C:51:GLU:HB2	2.02	0.40
1:A:183:ILE:HD11	1:A:267:ILE:CD1	2.51	0.40
4:H:95:GLU:O	4:H:96:GLU:HG2	2.22	0.40
1:C:404:ALA:C	1:C:406:PHE:N	2.74	0.40
1:A:168:ILE:HD11	1:A:329:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/510 (96%)	468 (96%)	19 (4%)	3 (1%)	33	47
1	B	490/510 (96%)	451 (92%)	31 (6%)	8 (2%)	14	18
1	C	490/510 (96%)	468 (96%)	21 (4%)	1 (0%)	56	74
2	D	465/482 (96%)	437 (94%)	27 (6%)	1 (0%)	56	74
2	E	464/482 (96%)	434 (94%)	23 (5%)	7 (2%)	15	20
2	F	464/482 (96%)	433 (93%)	27 (6%)	4 (1%)	25	35
3	G	257/272 (94%)	223 (87%)	26 (10%)	8 (3%)	7	5
4	H	129/146 (88%)	118 (92%)	8 (6%)	3 (2%)	10	10
5	I	45/50 (90%)	36 (80%)	4 (9%)	5 (11%)	1	0
All	All	3294/3444 (96%)	3068 (93%)	186 (6%)	40 (1%)	19	26

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	B	404	ALA
1	B	405	GLN
1	B	406	PHE
1	B	411	ASP
2	E	391	LEU
2	E	472	LYS
4	H	71	THR
5	I	29	GLU
1	A	488	LYS
1	C	407	GLY
2	F	28	GLY
2	F	246	GLN
2	F	385	GLN
3	G	51	LEU
3	G	56	ASP
1	A	21	THR

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Mol	Chain	Res	Type
1	B	408	SER
1	B	452	TYR
2	D	448	GLU
2	E	389	ALA
3	G	72	SER
3	G	180	SER
5	I	36	LYS
1	B	31	VAL
2	E	109	LYS
3	G	122	ASP
4	H	49	ALA
5	I	40	SER
1	B	400	VAL
2	E	394	ASP
2	E	455	GLN
3	G	116	LEU
3	G	179	PHE
3	G	185	SER
4	H	79	SER
5	I	28	THR
5	I	42	ILE
2	E	279	VAL
2	F	279	VAL

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	397/412 (96%)	380 (96%)	17 (4%)	40	59
1	B	397/412 (96%)	378 (95%)	19 (5%)	35	53
1	C	397/412 (96%)	374 (94%)	23 (6%)	28	43
2	D	377/386 (98%)	367 (97%)	10 (3%)	57	78
2	E	376/386 (97%)	359 (96%)	17 (4%)	38	57
2	F	376/386 (97%)	363 (96%)	13 (4%)	48	69
3	G	225/230 (98%)	210 (93%)	15 (7%)	23	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	104/109 (95%)	100 (96%)	4 (4%)	44	65
5	I	38/41 (93%)	35 (92%)	3 (8%)	18	26
All	All	2687/2774 (97%)	2566 (96%)	121 (4%)	38	57

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	50	GLU
1	A	52	MET
1	A	59	LEU
1	A	79	ASP
1	A	80	LYS
1	A	99	VAL
1	A	141	SER
1	A	143	ARG
1	A	164	ARG
1	A	168	ILE
1	A	371	VAL
1	A	438	ILE
1	A	444	VAL
1	A	469	LEU
1	A	479	LEU
1	A	493	SER
1	B	21	THR
1	B	30	ARG
1	B	99	VAL
1	B	146	MET
1	B	167	ILE
1	B	168	ILE
1	B	171	ARG
1	B	216	LEU
1	B	244	TYR
1	B	276	VAL
1	B	298	VAL
1	B	344	SER
1	B	371	VAL
1	B	384	LYS
1	B	400	VAL
1	B	406	PHE
1	B	449	VAL

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Mol	Chain	Res	Type
1	B	505	LEU
1	B	509	GLU
1	C	34	ILE
1	C	52	MET
1	C	56	SER
1	C	57	SER
1	C	64	LEU
1	C	74	VAL
1	C	91	THR
1	C	99	VAL
1	C	140	ILE
1	C	164	ARG
1	C	206	ILE
1	C	216	LEU
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN
1	C	381	ARG
1	C	408	SER
1	C	414	THR
1	C	434	SER
1	C	470	SER
1	C	479	LEU
1	C	485	THR
1	C	505	LEU
2	D	9	THR
2	D	61	ILE
2	D	97	VAL
2	D	132	ILE
2	D	250	ASP
2	D	258	ILE
2	D	274	ARG
2	D	282	GLN
2	D	335	LEU
2	D	384	LEU
2	E	9	THR
2	E	27	GLU
2	E	61	ILE
2	E	67	GLU
2	E	84	ILE
2	E	96	ASN
2	E	97	VAL

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Mol	Chain	Res	Type
2	E	139	VAL
2	E	151	LYS
2	E	223	ASN
2	E	232	VAL
2	E	252	LEU
2	E	257	ASN
2	E	258	ILE
2	E	282	GLN
2	E	391	LEU
2	E	431	LEU
2	F	51	GLN
2	F	76	LEU
2	F	96	ASN
2	F	97	VAL
2	F	139	VAL
2	F	223	ASN
2	F	232	VAL
2	F	274	ARG
2	F	282	GLN
2	F	420	VAL
2	F	436	GLU
2	F	444	ILE
2	F	463	ILE
3	G	35	GLU
3	G	67	LEU
3	G	110	ASP
3	G	113	ARG
3	G	118	ARG
3	G	125	LEU
3	G	126	VAL
3	G	130	GLU
3	G	180	SER
3	G	184	ILE
3	G	190	MET
3	G	205	GLN
3	G	212	ILE
3	G	213	ILE
3	G	262	LEU
4	H	54	THR
4	H	57	VAL
4	H	91	GLN
4	H	112	LEU

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Mol	Chain	Res	Type
5	I	37	THR
5	I	41	THR
5	I	42	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	379	GLN
1	A	396	GLN
1	A	405	GLN
1	A	477	GLN
1	B	65	ASN
1	B	186	GLN
1	B	349	GLN
1	B	466	ASN
1	B	475	GLN
1	B	503	ASN
1	C	48	GLN
1	C	215	GLN
1	C	260	ASN
1	C	263	HIS
1	C	349	GLN
1	C	416	GLN
1	C	432	GLN
2	D	130	GLN
2	D	194	ASN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	D	385	GLN
2	D	411	GLN
2	E	51	GLN
2	E	96	ASN
2	E	194	ASN
2	E	223	ASN
2	E	257	ASN
2	E	263	GLN
2	E	282	GLN
2	E	411	GLN
2	F	51	GLN
2	F	96	ASN

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Mol	Chain	Res	Type
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	419	GLN
2	F	443	GLN
3	G	82	HIS
3	G	88	GLN
3	G	225	GLN
3	G	234	ASN
4	H	91	GLN
4	H	111	ASN
4	H	132	GLN
5	I	16	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	A	600	7	33,33,33	0.77	0	52,52,52	0.76	0
8	ADP	B	600	7	29,29,29	0.82	0	45,45,45	0.81	0
9	GOL	B	701	-	5,5,5	0.31	0	5,5,5	0.38	0
6	ATP	C	600	7	33,33,33	0.90	0	52,52,52	0.84	0
8	ADP	D	600	7	29,29,29	0.87	0	45,45,45	0.81	0
10	DCW	D	700	2	17,17,17	1.01	0	21,21,21	1.18	2 (9%)
11	SO4	E	630	-	4,4,4	1.01	0	6,6,6	0.09	0
8	ADP	F	600	7	29,29,29	0.82	0	45,45,45	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	600	7	-	0/22/38/38	0/1/3/3
8	ADP	B	600	7	-	0/16/32/32	0/1/3/3
9	GOL	B	701	-	-	0/4/4/4	0/0/0/0
6	ATP	C	600	7	-	0/22/38/38	0/1/3/3
8	ADP	D	600	7	-	0/16/32/32	0/1/3/3
10	DCW	D	700	2	-	1/8/24/24	0/2/2/2
11	SO4	E	630	-	-	0/0/0/0	0/0/0/0
8	ADP	F	600	7	-	0/16/32/32	0/1/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	700	DCW	C8-N2-C1	2.68	130.15	123.21
10	D	700	DCW	C10-C9-C8	2.18	114.58	111.12

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	700	DCW	O1-C1-N1-C2

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	492/510 (96%)	-0.31	10 (2%) 62 59	32, 46, 74, 104	0
1	B	492/510 (96%)	-0.14	20 (4%) 35 33	32, 48, 95, 143	0
1	C	492/510 (96%)	-0.40	7 (1%) 72 71	30, 44, 63, 102	0
2	D	467/482 (96%)	-0.37	6 (1%) 74 73	31, 45, 69, 100	0
2	E	466/482 (96%)	0.03	27 (5%) 22 20	34, 54, 101, 132	0
2	F	466/482 (96%)	-0.34	8 (1%) 67 65	32, 44, 74, 89	0
3	G	263/272 (96%)	0.50	34 (12%) 4 4	36, 68, 116, 133	0
4	H	131/146 (89%)	1.12	20 (15%) 3 2	67, 97, 131, 136	0
5	I	47/50 (94%)	1.06	11 (23%) 1 1	58, 91, 127, 129	0
All	All	3316/3444 (96%)	-0.12	143 (4%) 34 32	30, 48, 102, 143	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	THR	8.8
2	E	473	LEU	8.1
1	B	19	ALA	8.1
1	B	400	VAL	7.9
2	E	474	ALA	7.6
1	C	407	GLY	7.5
1	B	20	ASP	7.1
2	E	390	ILE	6.9
2	E	472	LYS	6.7
1	A	19	ALA	6.5
4	H	71	THR	6.0
5	I	47	VAL	5.8
3	G	60	PRO	5.8
1	B	406	PHE	5.6
4	H	144	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	405	GLN	5.3
1	B	403	PHE	5.1
1	C	409	ASP	5.0
1	B	402	ALA	4.8
1	C	408	SER	4.8
5	I	35	MET	4.5
1	A	21	THR	4.5
1	A	20	ASP	4.4
1	B	358	TYR	4.4
2	F	248	GLY	4.3
3	G	199	ASP	4.3
2	E	424	PHE	4.3
1	C	193	THR	4.3
3	G	194	ASP	4.2
3	G	58	LYS	4.2
3	G	1	ALA	4.2
4	H	15	GLN	4.0
1	B	408	SER	3.8
5	I	46	LYS	3.8
3	G	101	LYS	3.8
4	H	45	PHE	3.7
1	B	193	THR	3.7
1	B	410	LEU	3.6
3	G	116	LEU	3.5
3	G	39	LYS	3.5
2	E	423	VAL	3.5
1	B	416	GLN	3.5
3	G	117	HIS	3.5
3	G	193	TYR	3.5
2	D	399	GLU	3.4
5	I	29	GLU	3.4
2	E	27	GLU	3.3
3	G	59	THR	3.3
3	G	122	ASP	3.3
4	H	69	ASP	3.3
2	E	394	ASP	3.3
3	G	180	SER	3.3
2	E	42	GLU	3.2
2	E	389	ALA	3.2
4	H	109	LYS	3.2
2	D	246	GLN	3.2
1	B	22	SER	3.1

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Mol	Chain	Res	Type	RSRZ
4	H	42	THR	3.1
2	D	248	GLY	3.1
5	I	28	THR	3.1
3	G	53	GLU	3.0
4	H	67	ALA	2.9
3	G	61	GLU	2.9
3	G	181	LEU	2.9
3	G	103	VAL	2.9
2	E	427	HIS	2.8
3	G	120	HIS	2.8
5	I	40	SER	2.8
2	D	28	GLY	2.8
2	F	246	GLN	2.8
3	G	56	ASP	2.7
1	B	404	ALA	2.7
5	I	36	LYS	2.6
3	G	195	ASP	2.6
2	D	249	GLN	2.6
2	E	111	LYS	2.6
2	E	386	ASP	2.6
5	I	30	PHE	2.6
1	A	457	GLU	2.6
4	H	34	ARG	2.6
1	C	406	PHE	2.6
3	G	184	ILE	2.6
3	G	36	ARG	2.5
1	A	22	SER	2.5
3	G	118	ARG	2.5
3	G	106	ILE	2.5
4	H	128	ARG	2.4
4	H	56	GLN	2.4
5	I	22	VAL	2.4
4	H	106	GLY	2.4
5	I	6	GLN	2.4
1	A	499	GLU	2.4
2	E	345	TYR	2.3
2	E	451	HIS	2.3
2	E	178	GLY	2.3
4	H	68	GLU	2.3
4	H	37	ASP	2.3
1	B	392	LEU	2.3
3	G	102	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	412	ALA	2.3
2	E	398	GLU	2.3
1	A	23	VAL	2.3
2	F	42	GLU	2.3
3	G	96	LEU	2.2
3	G	51	LEU	2.2
3	G	105	ILE	2.2
3	G	192	ILE	2.2
3	G	134	ARG	2.2
1	B	413	ALA	2.2
2	E	395	GLU	2.2
2	E	471	ASP	2.2
2	F	426	GLY	2.2
2	E	301	LYS	2.2
3	G	87	LYS	2.2
1	C	381	ARG	2.2
4	H	59	ARG	2.2
1	B	389	THR	2.2
2	E	425	THR	2.1
4	H	113	GLU	2.1
1	C	194	ASP	2.1
2	D	398	GLU	2.1
1	B	506	ALA	2.1
1	A	404	ALA	2.1
4	H	140	ALA	2.1
1	A	25	LEU	2.1
2	E	428	LEU	2.1
3	G	153	TYR	2.1
2	E	426	GLY	2.1
1	A	30	ARG	2.1
2	E	337	ARG	2.1
2	F	178	GLY	2.1
2	F	175	LYS	2.1
5	I	43	LYS	2.1
2	F	28	GLY	2.0
2	E	439	LYS	2.0
4	H	32	ASN	2.0
3	G	69	ILE	2.0
2	E	399	GLU	2.0
4	H	70	GLY	2.0
3	G	50	ALA	2.0
4	H	121	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	160	VAL	2.0
2	F	249	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	SO4	E	630	5/5	0.35	4.72	100,100,100,100	0
7	MG	C	601	1/1	0.15	4.52	43,43,43,43	0
7	MG	D	601	1/1	0.15	3.69	35,35,35,35	0
10	DCW	D	700	16/16	0.31	2.60	69,73,78,78	0
7	MG	F	601	1/1	0.10	0.70	34,34,34,34	0
9	GOL	B	701	6/6	0.11	-0.08	39,43,44,45	0
6	ATP	A	600	31/31	0.11	-0.20	42,44,56,56	0
6	ATP	C	600	31/31	0.11	-0.22	36,42,51,52	0
7	MG	A	601	1/1	0.11	-0.35	44,44,44,44	0
8	ADP	F	600	27/27	0.09	-0.62	41,42,45,45	0
8	ADP	D	600	27/27	0.09	-0.88	35,37,38,39	0
8	ADP	B	600	27/27	0.09	-1.22	44,52,56,56	0
7	MG	B	601	1/1	0.05	-3.59	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.