



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:33 PM GMT

PDB ID : 1G20
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 2.20 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>

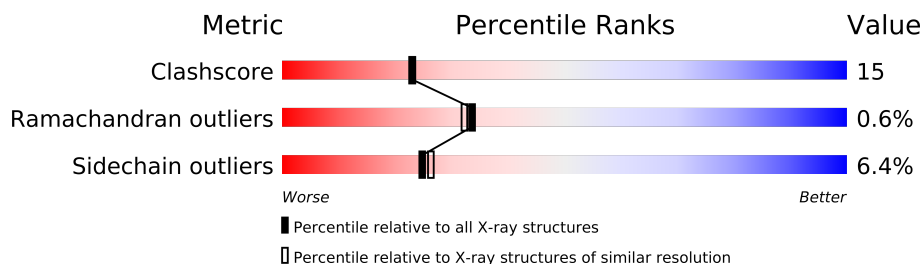
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.20 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	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	
1	C	492	
2	B	523	
2	D	523	
3	E	289	
3	F	289	
3	G	289	
3	H	289	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24903 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	259	Total	C	N	O	S	3	0	0
			1953	1227	330	376	20			
3	F	260	Total	C	N	O	S	0	0	0
			1952	1226	327	379	20			
3	G	257	Total	C	N	O	S	5	0	0
			1938	1219	327	372	20			
3	H	262	Total	C	N	O	S	3	0	0
			1984	1244	337	383	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	DELETION	UNP P00459
F	?	-	LEU	DELETION	UNP P00459
G	?	-	LEU	DELETION	UNP P00459

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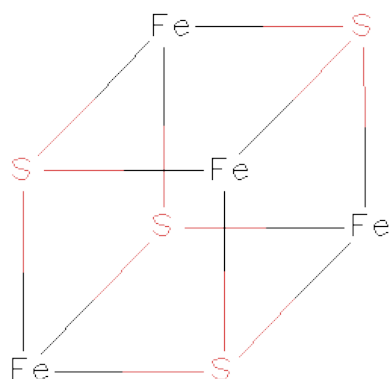
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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	DELETION	UNP P00459

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

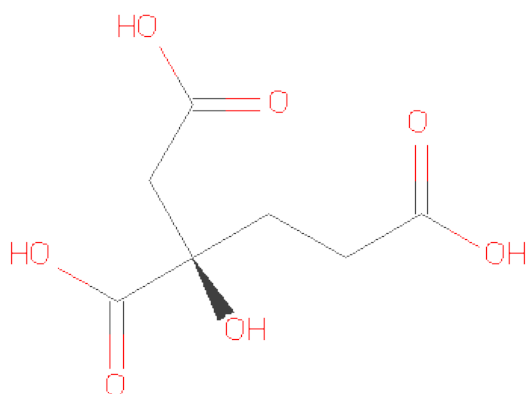
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



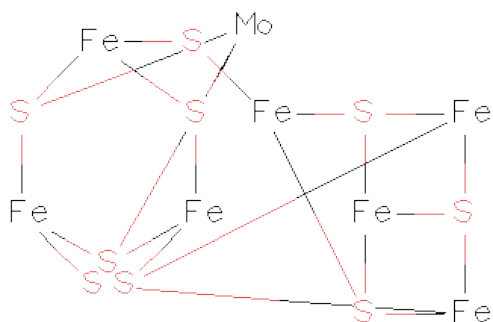
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Fe S 8 4 4	0	0
5	G	1	Total Fe S 8 4 4	0	0

- Molecule 6 is 3-HYDROXY-3-CARBOXY-ADIPIACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



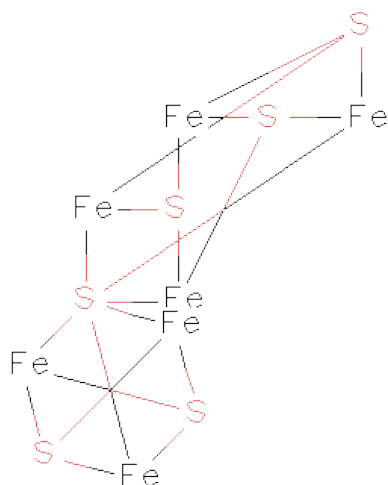
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			14	7	7		
6	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 7 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
7	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 8 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			15	8	7		
8	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	211	Total	O	0	0
			211	211		
9	B	309	Total	O	0	0
			309	309		
9	C	104	Total	O	0	0
			104	104		
9	D	235	Total	O	0	0
			235	235		
9	E	56	Total	O	0	0
			56	56		
9	F	62	Total	O	0	0
			62	62		
9	G	37	Total	O	0	0
			37	37		
9	H	52	Total	O	0	0
			52	52		

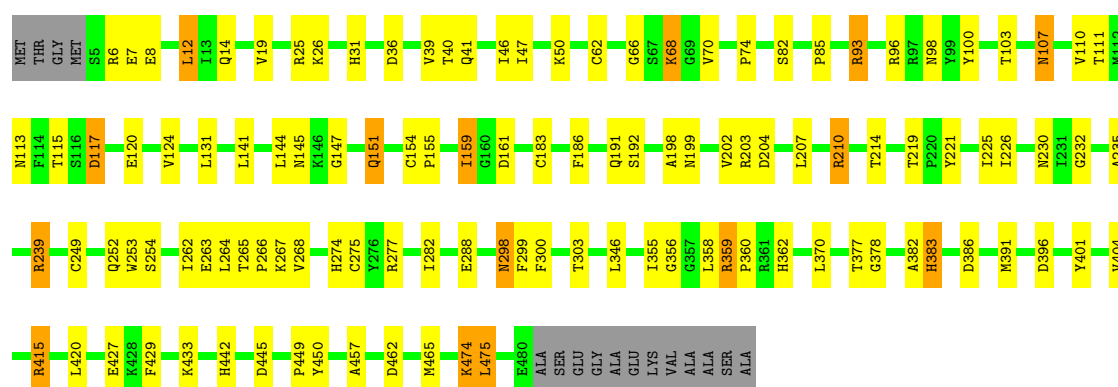
3 Residue-property plots

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.

Note EDS was not executed.

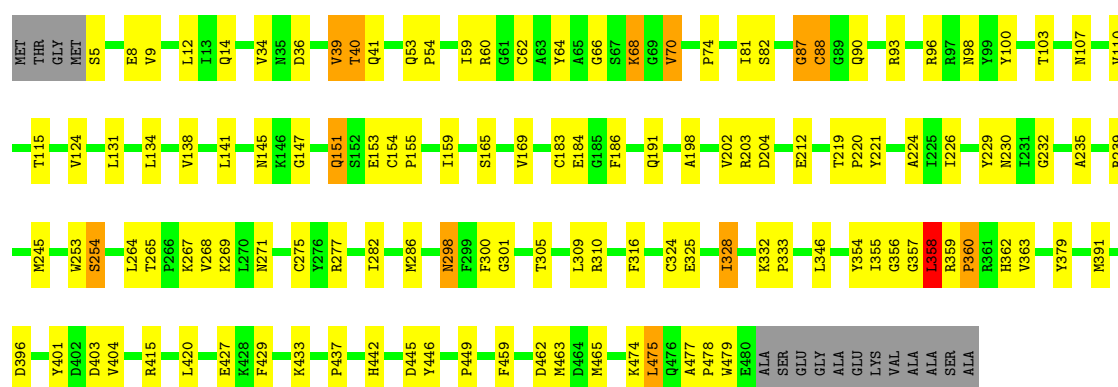
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

Chain A:



• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

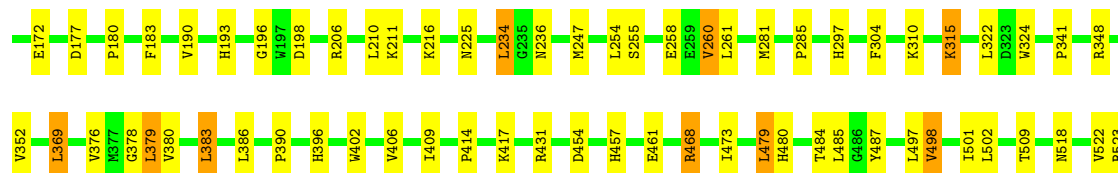
Chain C:



• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

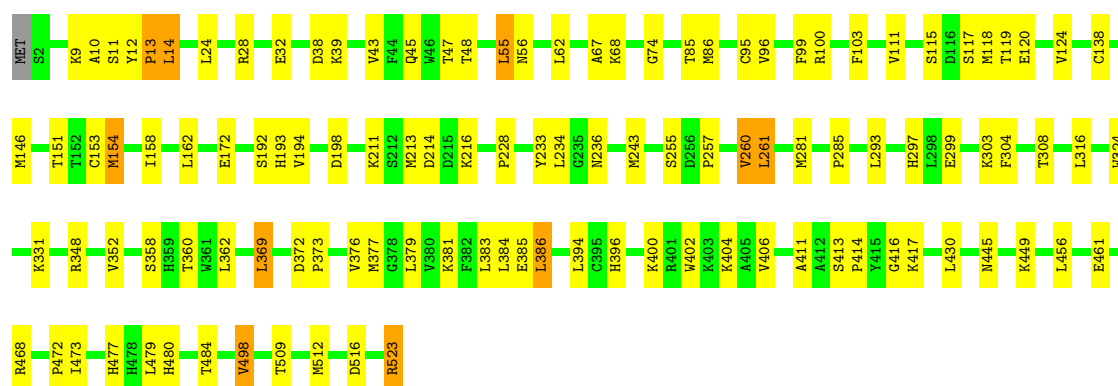
Chain B:





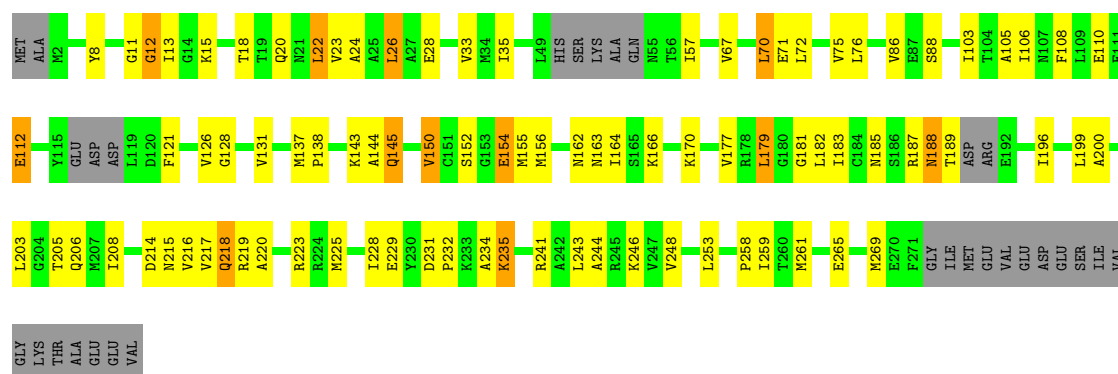
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

Chain D:



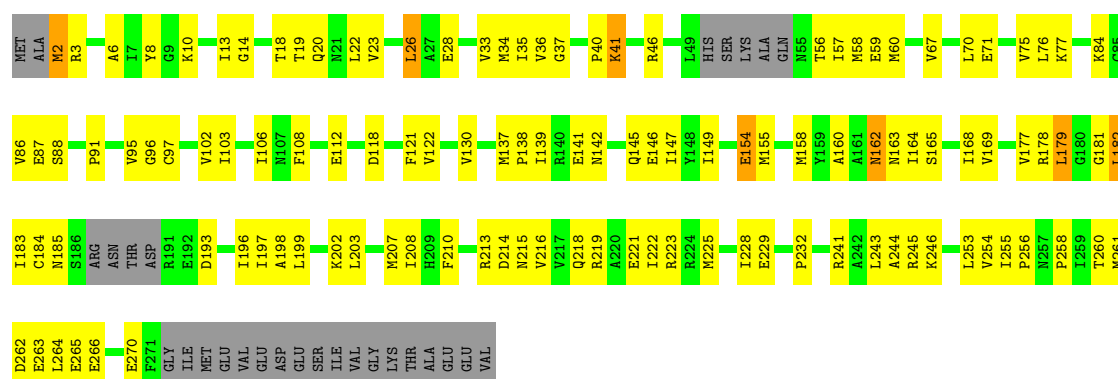
• Molecule 3: NITROGENASE IRON PROTEIN

Chain E:



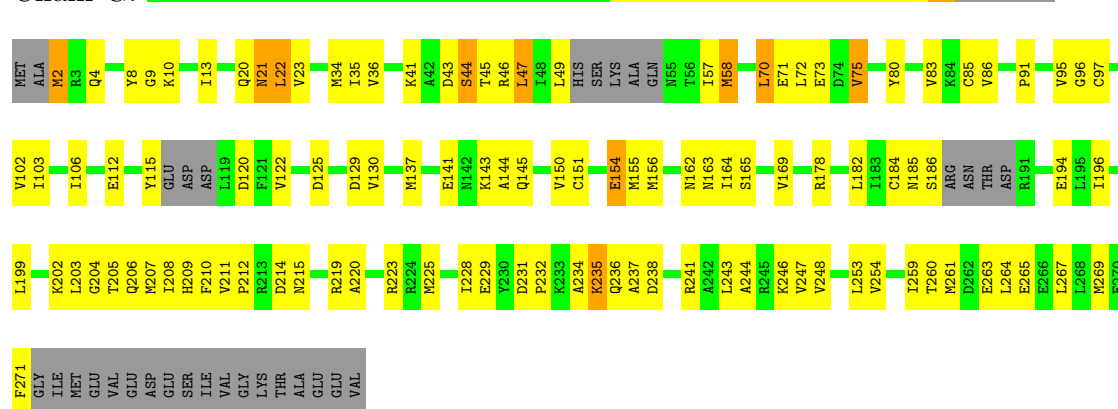
• Molecule 3: NITROGENASE IRON PROTEIN

Chain F:



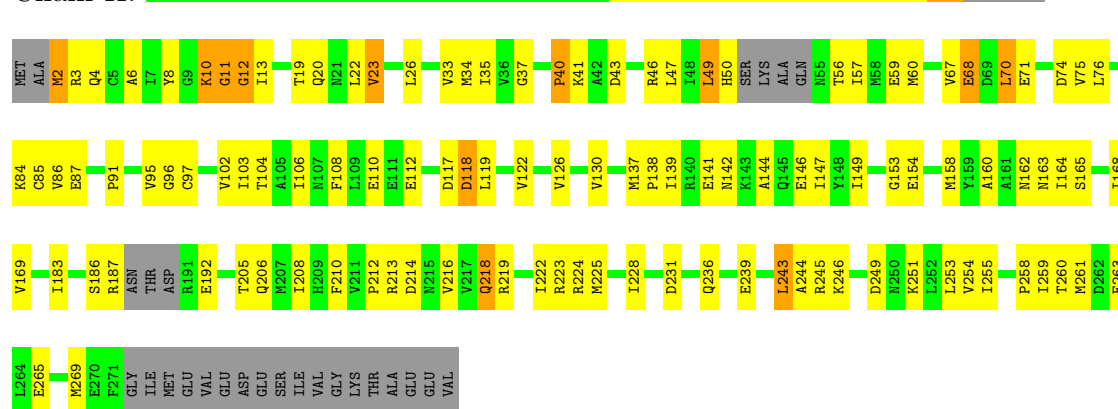
● Molecule 3: NITROGENASE IRON PROTEIN

Chain G:



● Molecule 3: NITROGENASE IRON PROTEIN

Chain H:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.24Å 111.46Å 121.59Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	89.1 (20.00-2.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24903	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CFM, CLF, CA, HCA

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	0.47	0/3864	0.87	4/5212 (0.1%)
1	C	0.49	0/3864	0.86	5/5212 (0.1%)
2	B	0.49	0/4280	0.82	3/5786 (0.1%)
2	D	0.44	0/4280	0.80	2/5786 (0.0%)
3	E	0.29	0/1973	0.63	0/2654
3	F	0.28	0/1973	0.62	0/2655
3	G	0.31	0/1958	0.60	1/2633 (0.0%)
3	H	0.32	0/2006	0.63	1/2699 (0.0%)
All	All	0.42	0/24198	0.77	16/32637 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	210	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	C	420	LEU	CA-CB-CG	6.50	130.26	115.30
1	A	420	LEU	CA-CB-CG	6.30	129.78	115.30
1	C	88	CYS	CA-CB-SG	-6.02	103.17	114.00
1	C	39	VAL	CB-CA-C	-5.96	100.07	111.40
2	B	12	TYR	N-CA-C	-5.47	96.23	111.00
2	B	498	VAL	CB-CA-C	-5.35	101.23	111.40
1	C	358	LEU	CA-CB-CG	5.24	127.34	115.30
3	G	207	MET	N-CA-C	-5.23	96.89	111.00
1	A	210	ARG	CB-CG-CD	5.22	125.16	111.60
2	D	12	TYR	N-CA-C	-5.13	97.16	111.00
2	D	213	MET	N-CA-C	5.12	124.82	111.00
1	C	475	LEU	CA-CB-CG	5.11	127.06	115.30
3	H	118	ASP	N-CA-C	5.11	124.80	111.00
2	B	260	VAL	CB-CA-C	-5.06	101.79	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3776	0	3708	86	0
1	C	3776	0	3708	98	0
2	B	4174	0	4087	59	0
2	D	4174	0	4087	76	0
3	E	1953	0	1971	72	0
3	F	1952	0	1958	98	0
3	G	1938	0	1958	115	0
3	H	1984	0	1993	143	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	E	8	0	0	0	0
5	G	8	0	0	0	0
6	A	14	0	6	3	0
6	C	14	0	6	2	0
7	A	17	0	0	5	0
7	C	17	0	0	6	0
8	B	15	0	0	1	0
8	D	15	0	0	1	0
9	A	211	0	0	6	0
9	B	309	0	0	6	0
9	C	104	0	0	1	0
9	D	235	0	0	6	0
9	E	56	0	0	2	0
9	F	62	0	0	0	0
9	G	37	0	0	0	0
9	H	52	0	0	3	0
All	All	24903	0	23482	692	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 15.

All (692) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:231:ASP:OD2	3:G:234:ALA:HB2	1.31	1.25
1:C:253:TRP:CZ3	1:C:282:ILE:HD13	1.78	1.16
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.28	1.14
3:F:23:VAL:HG21	3:F:35:ILE:HD11	1.32	1.04
3:G:23:VAL:HG21	3:G:35:ILE:HD11	1.40	1.01
1:A:210:ARG:HD3	1:A:263:GLU:CB	1.90	1.01
3:G:215:ASN:O	3:G:219:ARG:HG3	1.62	0.99
1:A:210:ARG:HD3	1:A:263:GLU:HB3	1.01	0.99
3:G:219:ARG:O	3:G:223:ARG:HD3	1.66	0.95
3:E:162:ASN:HD21	3:E:259:ILE:H	1.09	0.94
3:G:129:ASP:CG	3:H:41:LYS:NZ	2.21	0.94
1:C:39:VAL:HG23	1:C:391:MET:HG3	1.49	0.94
1:C:325:GLU:HA	1:C:328:ILE:CG2	1.99	0.93
1:C:253:TRP:HZ3	1:C:282:ILE:HD13	1.14	0.93
1:C:324:CYS:O	1:C:328:ILE:HG22	1.68	0.92
1:A:8:GLU:HA	1:A:8:GLU:OE1	1.70	0.90
1:A:359:ARG:HG3	7:A:1496:CFM:S3A	2.13	0.89
3:G:205:THR:HG23	3:G:206:GLN:H	1.38	0.88
1:A:210:ARG:CD	1:A:263:GLU:HB3	1.97	0.87
1:A:68:LYS:HB2	1:A:151:GLN:HG2	1.54	0.87
3:E:228:ILE:H	3:E:228:ILE:HD12	1.41	0.86
1:A:36:ASP:O	1:A:39:VAL:HG22	1.77	0.85
3:H:46:ARG:NH2	3:H:224:ARG:HE	1.75	0.84
3:G:129:ASP:CG	3:H:41:LYS:HZ3	1.78	0.84
3:H:118:ASP:C	3:H:119:LEU:HD12	1.99	0.83
3:E:57:ILE:HG12	3:E:75:VAL:HG21	1.59	0.83
3:H:154:GLU:HB2	3:H:187:ARG:NH1	1.93	0.83
1:A:210:ARG:HD2	1:A:263:GLU:OE2	1.79	0.83
3:E:23:VAL:HG21	3:E:35:ILE:HD11	1.59	0.82
3:G:231:ASP:OD2	3:G:234:ALA:CB	2.23	0.81
3:G:129:ASP:CB	3:H:41:LYS:HE2	2.12	0.80
3:G:205:THR:HG23	3:G:206:GLN:N	1.96	0.80
1:C:39:VAL:O	1:C:41:GLN:N	2.16	0.79
3:F:103:ILE:HA	3:F:137:MET:HG3	1.64	0.78
3:G:72:LEU:HB2	3:G:112:GLU:HG2	1.64	0.78
2:D:413:SER:O	2:D:417:LYS:HE3	1.83	0.77
3:H:76:LEU:HD23	3:H:86:VAL:HG22	1.65	0.77
3:G:228:ILE:HD12	3:G:228:ILE:H	1.48	0.77
2:D:118:MET:HE2	2:D:154:MET:SD	2.25	0.76
3:F:260:THR:HG22	3:F:262:ASP:H	1.51	0.76
1:C:221:TYR:HA	1:C:316:PHE:CE2	2.21	0.76
3:G:244:ALA:O	3:G:248:VAL:HG23	1.86	0.75
3:G:129:ASP:HB3	3:H:41:LYS:HE2	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:HIS:ND1	6:A:1494:HCA:H52	2.02	0.74
3:F:207:MET:HE1	3:F:210:PHE:HB2	1.69	0.74
3:F:182:LEU:HD21	3:F:199:LEU:HD12	1.68	0.74
3:H:219:ARG:O	3:H:222:ILE:HG12	1.88	0.73
1:A:275:CYS:HA	1:A:358:LEU:CD2	2.15	0.73
3:H:6:ALA:HB3	3:H:147:ILE:CD1	2.18	0.73
3:F:162:ASN:HD21	3:F:258:PRO:HA	1.51	0.73
1:C:81:ILE:HD13	1:C:134:LEU:HD21	1.69	0.72
3:G:8:TYR:HB3	3:G:164:ILE:HD13	1.71	0.72
2:B:216:LYS:HG2	2:B:285:PRO:HB2	1.70	0.72
2:D:304:PHE:O	2:D:308:THR:HB	1.90	0.72
3:H:265:GLU:O	3:H:269:MET:HG2	1.90	0.72
3:H:139:ILE:HG22	3:H:147:ILE:HD11	1.72	0.71
1:C:39:VAL:HG21	1:C:391:MET:CE	2.20	0.71
3:H:8:TYR:HB3	3:H:164:ILE:HD13	1.70	0.71
1:A:7:GLU:OE1	1:A:7:GLU:N	2.23	0.71
3:G:129:ASP:OD2	3:H:41:LYS:HD3	1.91	0.70
1:C:253:TRP:CH2	1:C:282:ILE:HD13	2.27	0.70
3:G:129:ASP:HB2	3:H:41:LYS:HZ1	1.56	0.70
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.73	0.70
1:A:68:LYS:C	1:A:68:LYS:HD2	2.12	0.70
3:E:162:ASN:HD21	3:E:259:ILE:N	1.89	0.70
3:H:154:GLU:HB2	3:H:187:ARG:HH12	1.55	0.69
1:A:31:HIS:O	1:A:46:ILE:HD11	1.92	0.69
2:D:362:LEU:HD13	2:D:386:LEU:HG	1.72	0.69
3:G:44:SER:HB3	3:G:125:ASP:OD2	1.93	0.69
3:G:231:ASP:CG	3:G:231:ASP:O	2.30	0.69
3:E:228:ILE:HD12	3:E:228:ILE:N	2.08	0.68
1:C:298:ASN:HD21	1:C:300:PHE:HB2	1.58	0.68
3:H:2:MET:HE2	3:H:3:ARG:N	2.09	0.68
1:C:310:ARG:NH1	1:C:328:ILE:HD13	2.09	0.67
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.77	0.67
3:F:266:GLU:O	3:F:270:GLU:HG3	1.95	0.67
3:G:208:ILE:O	3:G:246:LYS:HD3	1.94	0.67
3:H:10:LYS:HE2	3:H:10:LYS:HA	1.77	0.67
1:A:415:ARG:HA	1:A:415:ARG:NE	2.09	0.67
3:G:237:ALA:O	3:G:241:ARG:HG3	1.94	0.67
2:B:473:ILE:HD12	2:B:479:LEU:HD23	1.77	0.67
3:G:22:LEU:HG	3:G:243:LEU:HD22	1.76	0.67
1:A:232:GLY:O	1:A:449:PRO:HD3	1.95	0.67
3:E:217:VAL:HB	3:E:218:GLN:OE1	1.94	0.67
1:A:230:ASN:HD22	1:A:235:ALA:H	1.42	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:146:GLU:HG2	3:F:253:LEU:HD11	1.76	0.66
1:C:39:VAL:CG2	1:C:391:MET:HG3	2.23	0.66
3:G:49:LEU:HD11	3:G:85:CYS:SG	2.35	0.66
3:G:243:LEU:O	3:G:247:VAL:HG23	1.95	0.66
3:E:155:MET:HG2	3:F:221:GLU:OE2	1.96	0.66
1:A:103:THR:H	1:A:107:ASN:HD21	1.43	0.65
3:F:13:ILE:HG22	3:F:185:ASN:HD22	1.60	0.65
1:C:229:TYR:CE1	7:C:3496:CFM:S2A	2.89	0.65
3:G:162:ASN:HD21	3:G:259:ILE:H	1.45	0.65
3:G:129:ASP:OD2	3:H:41:LYS:CE	2.45	0.65
2:B:414:PRO:HA	2:B:417:LYS:HD2	1.78	0.65
2:B:348:ARG:HG3	2:B:487:TYR:CE2	2.32	0.65
3:F:76:LEU:HD23	3:F:86:VAL:HG13	1.80	0.64
1:A:219:THR:HG22	1:A:221:TYR:H	1.62	0.64
3:G:129:ASP:CB	3:H:41:LYS:CE	2.75	0.64
1:C:220:PRO:O	1:C:316:PHE:HE2	1.81	0.64
1:A:442:HIS:CG	6:A:1494:HCA:H52	2.33	0.64
3:E:228:ILE:CD1	3:E:228:ILE:H	2.10	0.64
1:C:232:GLY:O	1:C:449:PRO:HD3	1.98	0.64
3:H:95:VAL:HG22	3:H:96:GLY:H	1.63	0.63
1:C:159:ILE:HG13	3:H:97:CYS:HB2	1.80	0.63
3:H:254:VAL:HG22	3:H:255:ILE:N	2.12	0.63
3:E:18:THR:HG21	3:E:185:ASN:OD1	1.99	0.63
3:F:214:ASP:OD2	3:F:216:VAL:HG23	1.98	0.63
1:C:40:THR:O	1:C:40:THR:HG22	1.99	0.63
3:H:10:LYS:HE2	3:H:11:GLY:H	1.62	0.63
3:G:129:ASP:CB	3:H:41:LYS:NZ	2.61	0.63
3:F:254:VAL:HG12	3:F:255:ILE:N	2.12	0.63
3:H:261:MET:O	3:H:265:GLU:HG3	1.99	0.62
3:G:2:MET:CE	3:G:122:VAL:HG23	2.28	0.62
3:H:10:LYS:HG2	3:H:160:ALA:CB	2.30	0.62
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.81	0.62
3:G:36:VAL:HA	3:G:86:VAL:HG23	1.80	0.62
1:C:36:ASP:O	1:C:39:VAL:HG13	1.99	0.62
3:F:262:ASP:O	3:F:266:GLU:HG3	2.00	0.62
2:D:360:THR:HB	9:D:3531:HOH:O	1.98	0.62
2:D:86:MET:HG2	2:D:138:CYS:SG	2.40	0.62
1:C:68:LYS:HB2	1:C:151:GLN:HG2	1.81	0.62
1:A:145:ASN:HD22	1:A:147:GLY:H	1.47	0.62
3:E:57:ILE:CG1	3:E:75:VAL:HG21	2.29	0.62
3:G:129:ASP:CB	3:H:41:LYS:HZ1	2.13	0.62
3:H:56:THR:HG23	3:H:59:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:20:GLN:HA	3:F:23:VAL:HG22	1.82	0.62
3:E:15:LYS:HG2	3:E:150:VAL:HG11	1.80	0.62
1:C:39:VAL:HG21	1:C:391:MET:HE3	1.80	0.61
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.82	0.61
3:H:210:PHE:O	3:H:212:PRO:HD3	2.00	0.61
3:H:43:ASP:OD2	3:H:46:ARG:HB2	2.00	0.61
1:A:415:ARG:CA	1:A:415:ARG:NE	2.61	0.61
3:G:260:THR:HG23	3:G:263:GLU:H	1.64	0.61
3:F:198:ALA:O	3:F:202:LYS:HG2	2.00	0.61
3:G:129:ASP:OD2	3:H:41:LYS:NZ	2.33	0.61
2:D:299:GLU:O	2:D:303:LYS:HG3	2.01	0.61
3:H:223:ARG:O	3:H:225:MET:HG2	2.00	0.61
3:H:10:LYS:HG2	3:H:160:ALA:HB2	1.83	0.61
3:H:95:VAL:HG22	3:H:96:GLY:N	2.16	0.61
3:H:102:VAL:O	3:H:106:ILE:HG12	2.01	0.61
1:C:103:THR:H	1:C:107:ASN:HD21	1.47	0.61
1:C:442:HIS:CG	6:C:3494:HCA:H52	2.35	0.61
3:E:103:ILE:HG12	3:E:137:MET:HG3	1.83	0.61
2:B:67:ALA:H	2:B:396:HIS:HD2	1.49	0.61
1:A:66:GLY:O	1:A:70:VAL:HG22	2.01	0.60
1:A:442:HIS:HB2	9:A:1509:HOH:O	1.99	0.60
1:A:68:LYS:HD2	1:A:68:LYS:O	2.01	0.60
3:H:22:LEU:HD23	3:H:26:LEU:HD13	1.83	0.60
3:F:179:LEU:HD22	3:F:181:GLY:H	1.65	0.60
1:C:221:TYR:HA	1:C:316:PHE:HE2	1.65	0.60
1:C:359:ARG:NH1	7:C:3496:CFM:S4B	2.74	0.60
3:F:40:PRO:HG2	3:F:41:LYS:HD3	1.82	0.60
1:A:207:LEU:HD22	1:A:282:ILE:HD11	1.83	0.60
3:F:260:THR:HB	3:F:263:GLU:HG3	1.82	0.60
3:E:162:ASN:ND2	3:E:259:ILE:H	1.91	0.60
1:C:275:CYS:HA	1:C:358:LEU:HG	1.84	0.60
3:H:103:ILE:HA	3:H:137:MET:HE3	1.84	0.59
3:E:15:LYS:HG2	3:E:150:VAL:CG1	2.32	0.59
3:G:260:THR:CG2	3:G:263:GLU:HG3	2.31	0.59
1:C:64:TYR:CE2	1:C:88:CYS:HB3	2.37	0.59
1:C:230:ASN:HD22	1:C:235:ALA:H	1.48	0.59
2:D:216:LYS:HG2	2:D:285:PRO:HB2	1.84	0.59
3:G:228:ILE:HD12	3:G:228:ILE:N	2.15	0.59
3:G:102:VAL:O	3:G:106:ILE:HG12	2.02	0.59
3:F:28:GLU:OE1	3:F:241:ARG:HD3	2.03	0.59
1:C:124:VAL:O	3:H:91:PRO:HB3	2.02	0.59
3:G:231:ASP:OD1	3:G:231:ASP:O	2.21	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:119:LEU:HD12	3:H:119:LEU:N	2.17	0.59
3:H:57:ILE:HD11	3:H:86:VAL:HG11	1.85	0.59
3:G:202:LYS:HG3	3:G:267:LEU:HD11	1.85	0.59
1:C:325:GLU:O	1:C:328:ILE:HG23	2.02	0.58
1:C:442:HIS:HB2	9:C:3565:HOH:O	2.03	0.58
3:E:219:ARG:O	3:E:223:ARG:HD3	2.02	0.58
2:D:304:PHE:CZ	2:D:308:THR:HG21	2.38	0.58
3:G:10:LYS:NZ	3:G:156:MET:HB3	2.18	0.58
3:E:76:LEU:HD23	3:E:86:VAL:HG13	1.85	0.58
3:E:12:GLY:H	3:F:10:LYS:HZ2	1.52	0.58
3:G:228:ILE:H	3:G:228:ILE:CD1	2.16	0.58
3:F:6:ALA:HB3	3:F:147:ILE:CD1	2.34	0.58
3:G:71:GLU:HG3	3:G:73:GLU:OE1	2.04	0.58
2:D:304:PHE:CE1	2:D:308:THR:HG21	2.39	0.58
1:A:415:ARG:HA	1:A:415:ARG:CZ	2.34	0.58
2:B:468:ARG:HB3	2:B:473:ILE:HD13	1.86	0.57
1:C:96:ARG:HD2	7:C:3496:CFM:S3B	2.44	0.57
1:C:141:LEU:HD21	2:D:56:ASN:HA	1.86	0.57
3:G:21:ASN:HD22	3:G:21:ASN:N	1.99	0.57
1:C:298:ASN:HD22	1:C:300:PHE:H	1.52	0.57
3:F:102:VAL:O	3:F:106:ILE:HG12	2.04	0.57
3:H:23:VAL:HG21	3:H:35:ILE:HD11	1.87	0.57
3:E:225:MET:HE1	3:E:229:GLU:HG2	1.85	0.57
3:G:235:LYS:HA	3:G:235:LYS:HE2	1.87	0.57
3:H:146:GLU:HG2	3:H:253:LEU:HD21	1.86	0.57
1:C:253:TRP:CZ3	1:C:282:ILE:CD1	2.71	0.57
3:F:179:LEU:HD12	3:F:256:PRO:HB3	1.86	0.57
3:G:2:MET:HE3	3:G:122:VAL:HG23	1.86	0.57
2:D:372:ASP:O	2:D:376:VAL:HG12	2.05	0.57
3:E:179:LEU:HD22	3:E:181:GLY:H	1.70	0.57
3:H:228:ILE:H	3:H:228:ILE:HD12	1.70	0.56
1:C:325:GLU:HA	1:C:328:ILE:HG21	1.81	0.56
3:H:23:VAL:HG11	3:H:35:ILE:HD11	1.86	0.56
3:H:162:ASN:HD21	3:H:259:ILE:H	1.51	0.56
3:G:129:ASP:CG	3:H:41:LYS:CE	2.74	0.56
3:H:26:LEU:HD12	3:H:244:ALA:HB1	1.88	0.56
3:H:6:ALA:HB3	3:H:147:ILE:HD12	1.87	0.56
3:G:129:ASP:OD2	3:H:41:LYS:CD	2.54	0.56
3:G:41:LYS:NZ	3:H:41:LYS:HZ1	2.04	0.56
3:H:218:GLN:O	3:H:222:ILE:HG23	2.05	0.56
3:F:76:LEU:HD22	3:F:84:LYS:HB3	1.87	0.56
1:A:93:ARG:HD2	1:A:111:THR:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:117:ASP:O	3:H:119:LEU:HD13	2.06	0.56
3:E:214:ASP:CG	3:E:216:VAL:HG22	2.27	0.56
3:H:46:ARG:NH2	3:H:224:ARG:NE	2.50	0.56
2:D:414:PRO:O	2:D:417:LYS:HG2	2.06	0.55
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.40	0.55
3:E:106:ILE:HD11	3:E:138:PRO:HG3	1.87	0.55
2:D:417:LYS:N	2:D:417:LYS:HE2	2.21	0.55
2:D:198:ASP:HB2	2:D:297:HIS:O	2.05	0.55
3:F:228:ILE:H	3:F:228:ILE:HD12	1.71	0.55
2:B:236:ASN:HB3	2:B:485:LEU:HD22	1.87	0.55
3:H:57:ILE:CG1	3:H:75:VAL:HG21	2.37	0.55
2:D:358:SER:HB3	2:D:498:VAL:HG11	1.88	0.55
3:G:165:SER:O	3:G:169:VAL:HG23	2.06	0.55
2:D:124:VAL:HG11	3:G:58:MET:HG2	1.89	0.55
3:F:77:LYS:HB3	3:F:77:LYS:NZ	2.22	0.55
3:H:214:ASP:OD2	3:H:216:VAL:HG23	2.05	0.55
3:H:117:ASP:OD1	3:H:119:LEU:HD11	2.07	0.55
3:H:228:ILE:N	3:H:228:ILE:HD12	2.22	0.55
1:C:298:ASN:ND2	1:C:300:PHE:H	2.05	0.55
3:F:36:VAL:HA	3:F:86:VAL:HG23	1.88	0.55
1:C:325:GLU:CA	1:C:328:ILE:CG2	2.82	0.54
3:F:178:ARG:HB2	3:F:253:LEU:HB3	1.89	0.54
3:H:146:GLU:HG2	3:H:253:LEU:CD2	2.37	0.54
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.43	0.54
3:G:46:ARG:HG3	3:G:46:ARG:HH11	1.71	0.54
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.89	0.54
3:G:261:MET:HG2	3:H:46:ARG:NH2	2.22	0.54
1:C:219:THR:HG22	1:C:221:TYR:H	1.72	0.54
3:E:231:ASP:OD2	3:E:234:ALA:HB2	2.07	0.54
3:F:225:MET:HE1	3:F:229:GLU:HG2	1.90	0.54
3:F:23:VAL:HG21	3:F:35:ILE:CD1	2.22	0.54
2:B:383:LEU:HD23	2:B:390:PRO:HB3	1.90	0.54
3:F:160:ALA:O	3:F:164:ILE:HG13	2.08	0.54
3:G:215:ASN:C	3:G:219:ARG:HG3	2.29	0.54
3:F:199:LEU:O	3:F:203:LEU:HD13	2.07	0.54
3:F:95:VAL:HG22	3:F:96:GLY:H	1.72	0.54
1:C:442:HIS:CE1	7:C:3496:CFM:S1B	3.02	0.53
3:E:182:LEU:O	3:E:208:ILE:HG22	2.08	0.53
1:A:25:ARG:NH1	1:A:26:LYS:HG2	2.24	0.53
3:G:184:CYS:SG	3:G:196:ILE:HG13	2.48	0.53
3:E:72:LEU:HB2	3:E:112:GLU:HG2	1.89	0.53
2:B:43:VAL:O	2:B:47:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:45:THR:O	3:G:49:LEU:HD13	2.09	0.53
3:H:23:VAL:HB	3:H:33:VAL:HG11	1.91	0.53
3:E:26:LEU:HD12	3:E:244:ALA:HB1	1.91	0.53
3:F:178:ARG:CB	3:F:253:LEU:HB3	2.39	0.53
1:A:214:THR:HA	9:A:1659:HOH:O	2.08	0.53
1:C:39:VAL:HG21	1:C:391:MET:HE2	1.91	0.53
3:G:204:GLY:O	3:G:254:VAL:HG21	2.09	0.53
1:C:60:ARG:HD2	1:C:403:ASP:OD2	2.08	0.53
2:D:118:MET:CE	2:D:154:MET:SD	2.96	0.52
3:E:170:LYS:HB2	3:E:170:LYS:NZ	2.24	0.52
3:H:2:MET:CE	3:H:122:VAL:HG23	2.39	0.52
3:F:254:VAL:CG1	3:F:255:ILE:N	2.72	0.52
3:G:260:THR:HG22	3:G:263:GLU:HG3	1.92	0.52
3:H:103:ILE:HG12	3:H:137:MET:HG3	1.90	0.52
2:D:119:THR:HG22	2:D:120:GLU:N	2.24	0.52
1:C:226:ILE:HA	1:C:253:TRP:HB2	1.91	0.52
3:G:205:THR:CG2	3:G:206:GLN:H	2.07	0.52
1:A:230:ASN:HD22	1:A:235:ALA:N	2.07	0.52
3:G:154:GLU:OE1	3:G:155:MET:N	2.32	0.52
1:C:245:MET:SD	1:C:309:LEU:HD22	2.49	0.52
3:H:40:PRO:HD3	9:H:320:HOH:O	2.10	0.52
1:C:62:CYS:O	1:C:191:GLN:HA	2.10	0.52
3:E:269:MET:HG3	3:F:222:ILE:HG21	1.90	0.52
3:H:60:MET:CE	3:H:74:ASP:HB3	2.39	0.52
1:C:74:PRO:HB2	1:C:254:SER:HB3	1.91	0.52
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.91	0.52
1:C:265:THR:O	1:C:268:VAL:HG22	2.09	0.52
1:A:275:CYS:CA	1:A:358:LEU:HD22	2.20	0.52
3:G:260:THR:HG22	3:G:263:GLU:OE2	2.10	0.52
3:E:131:VAL:CG1	3:F:41:LYS:HD2	2.39	0.52
1:A:265:THR:O	1:A:268:VAL:HG22	2.10	0.52
3:F:154:GLU:OE1	3:F:155:MET:N	2.42	0.52
1:C:141:LEU:HD11	2:D:55:LEU:HB3	1.90	0.52
3:H:245:ARG:HH11	3:H:245:ARG:HG3	1.75	0.52
3:F:57:ILE:HG12	3:F:75:VAL:HG21	1.91	0.52
3:H:117:ASP:OD1	3:H:119:LEU:CD1	2.58	0.51
3:H:106:ILE:O	3:H:110:GLU:HG2	2.11	0.51
3:E:244:ALA:O	3:E:248:VAL:HG23	2.10	0.51
1:A:12:LEU:HG	1:A:415:ARG:HG2	1.91	0.51
1:C:253:TRP:CH2	1:C:282:ILE:CD1	2.92	0.51
3:H:260:THR:OG1	3:H:263:GLU:HG3	2.10	0.51
3:E:33:VAL:HG13	3:E:121:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:205:THR:HG23	3:H:206:GLN:N	2.25	0.51
3:G:4:GLN:HB2	3:G:144:ALA:HA	1.91	0.51
3:E:235:LYS:HE2	3:E:235:LYS:HA	1.93	0.51
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.92	0.51
2:B:74:GLY:HA3	2:B:193:HIS:O	2.10	0.51
3:H:46:ARG:HH11	3:H:46:ARG:HG3	1.76	0.51
1:C:151:GLN:HG3	1:C:183:CYS:SG	2.50	0.51
1:A:429:PHE:O	1:A:433:LYS:HD3	2.11	0.51
3:F:182:LEU:CD2	3:F:199:LEU:HD12	2.41	0.51
3:F:183:ILE:HG12	3:F:208:ILE:CG2	2.41	0.51
2:B:100:ARG:HD2	2:B:111:VAL:O	2.09	0.51
1:C:90:GLN:HG3	2:D:68:LYS:O	2.11	0.51
1:A:355:ILE:HG22	1:A:356:GLY:H	1.75	0.51
3:H:2:MET:HE3	3:H:122:VAL:HG23	1.93	0.51
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.76	0.51
2:B:86:MET:HG2	2:B:138:CYS:SG	2.51	0.51
2:D:68:LYS:HE2	2:D:396:HIS:CE1	2.45	0.50
3:H:154:GLU:O	3:H:158:MET:HG3	2.11	0.50
3:H:187:ARG:HA	3:H:213:ARG:CZ	2.42	0.50
3:H:249:ASP:O	3:H:251:LYS:HD2	2.11	0.50
3:E:145:GLN:N	3:E:145:GLN:HE21	2.08	0.50
3:F:34:MET:HE1	3:F:76:LEU:HD11	1.91	0.50
3:G:129:ASP:CG	3:H:41:LYS:HZ1	2.10	0.50
3:H:60:MET:HB3	3:H:70:LEU:HD21	1.93	0.50
3:G:41:LYS:HZ3	3:H:41:LYS:HZ1	1.59	0.50
1:A:39:VAL:HG21	1:A:391:MET:HE3	1.93	0.50
3:H:164:ILE:O	3:H:168:ILE:HG13	2.12	0.50
3:G:10:LYS:HZ1	3:G:156:MET:HB3	1.77	0.50
2:B:163:ASN:HD22	2:B:183:PHE:HE2	1.58	0.50
2:B:376:VAL:O	2:B:380:VAL:HG23	2.12	0.50
2:D:45:GLN:O	2:D:48:THR:HB	2.12	0.50
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.93	0.50
2:B:3:GLN:NE2	2:B:9:LYS:H	2.10	0.50
3:E:22:LEU:O	3:E:22:LEU:HD22	2.11	0.50
3:G:155:MET:HE1	3:G:264:LEU:HD23	1.94	0.50
3:F:76:LEU:CD2	3:F:86:VAL:HG13	2.41	0.50
3:H:23:VAL:CG2	3:H:35:ILE:HD11	2.42	0.50
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.27	0.50
1:A:198:ALA:O	1:A:202:VAL:HG23	2.12	0.50
2:B:315:LYS:C	2:B:315:LYS:HD2	2.31	0.50
1:C:220:PRO:HA	1:C:269:LYS:HE2	1.93	0.50
1:C:359:ARG:O	1:C:363:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:301:GLY:O	1:C:305:THR:OG1	2.25	0.50
3:F:2:MET:HE3	3:F:122:VAL:HG23	1.94	0.50
3:E:154:GLU:OE1	3:E:155:MET:N	2.45	0.49
3:E:183:ILE:HG12	3:E:208:ILE:CG2	2.42	0.49
3:H:37:GLY:HA3	3:H:87:GLU:OE2	2.12	0.49
2:D:243:MET:HE3	9:D:3722:HOH:O	2.12	0.49
3:G:95:VAL:HG22	3:G:96:GLY:H	1.77	0.49
3:H:57:ILE:HG12	3:H:75:VAL:HG21	1.92	0.49
1:A:159:ILE:HG13	3:F:97:CYS:HB2	1.94	0.49
3:H:141:GLU:O	3:H:142:ASN:HB2	2.11	0.49
2:D:257:PRO:HB2	2:D:261:LEU:HD22	1.94	0.49
3:H:23:VAL:CG1	3:H:35:ILE:HD11	2.42	0.49
2:B:85:THR:HG22	2:B:146:MET:HB3	1.94	0.49
1:A:226:ILE:HA	1:A:253:TRP:HB2	1.93	0.49
1:A:100:TYR:CE2	1:A:110:VAL:HB	2.47	0.49
3:F:215:ASN:O	3:F:219:ARG:HG3	2.12	0.49
3:E:28:GLU:OE1	3:E:241:ARG:NH1	2.39	0.49
1:C:90:GLN:OE1	1:C:90:GLN:HA	2.10	0.49
1:C:459:PHE:O	1:C:463:MET:HG2	2.12	0.49
2:B:211:LYS:HG3	9:B:1631:HOH:O	2.11	0.49
1:A:96:ARG:HD2	7:A:1496:CFM:S3B	2.52	0.49
3:F:260:THR:HG22	3:F:261:MET:N	2.28	0.49
3:H:254:VAL:CG2	3:H:255:ILE:N	2.74	0.49
1:C:87:GLY:HA3	8:D:3498:CLF:S2B	2.53	0.49
3:G:231:ASP:O	3:G:232:PRO:C	2.51	0.49
3:F:6:ALA:HB3	3:F:147:ILE:HD12	1.93	0.49
3:G:49:LEU:N	3:G:49:LEU:HD12	2.28	0.49
1:A:85:PRO:HB2	8:B:1498:CLF:S2B	2.53	0.49
1:C:328:ILE:O	1:C:328:ILE:HG13	2.13	0.49
1:A:239:ARG:HG3	2:B:23:MET:SD	2.53	0.49
3:G:225:MET:SD	3:G:229:GLU:OE2	2.71	0.49
3:G:41:LYS:HZ2	3:H:41:LYS:NZ	2.11	0.49
3:E:269:MET:HE3	3:F:223:ARG:CZ	2.43	0.49
2:B:431:ARG:HD2	2:B:454:ASP:OD1	2.13	0.49
2:B:45:GLN:O	2:B:48:THR:HB	2.13	0.49
1:C:230:ASN:HD22	1:C:235:ALA:N	2.10	0.48
2:D:100:ARG:HD2	2:D:111:VAL:O	2.13	0.48
3:F:26:LEU:CD1	3:F:244:ALA:HB1	2.43	0.48
2:B:522:VAL:HG23	1:C:446:TYR:CE2	2.48	0.48
2:D:324:TRP:CE2	2:D:381:LYS:HD2	2.48	0.48
2:D:400:LYS:O	2:D:404:LYS:HG2	2.13	0.48
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:85:THR:HG22	2:D:146:MET:HB3	1.95	0.48
1:A:277:ARG:HD3	1:A:277:ARG:O	2.13	0.48
3:H:103:ILE:HA	3:H:137:MET:HG3	1.95	0.48
3:E:106:ILE:CG2	3:E:143:LYS:HZ1	2.27	0.48
3:E:12:GLY:N	3:F:10:LYS:HE3	2.29	0.48
3:G:103:ILE:HG12	3:G:137:MET:HG3	1.95	0.48
1:C:184:GLU:HG3	1:C:186:PHE:CZ	2.49	0.48
1:C:253:TRP:HZ3	1:C:282:ILE:CD1	2.05	0.48
3:H:108:PHE:CZ	3:H:112:GLU:HG3	2.49	0.48
3:H:126:VAL:HG22	3:H:138:PRO:HG2	1.95	0.48
3:H:22:LEU:O	3:H:26:LEU:HD13	2.14	0.48
3:G:2:MET:HE2	3:G:120:ASP:O	2.13	0.48
2:B:234:LEU:HD22	2:B:480:HIS:HD2	1.79	0.48
3:F:184:CYS:SG	3:F:196:ILE:HG13	2.54	0.48
3:G:41:LYS:NZ	3:G:129:ASP:OD1	2.47	0.47
1:C:81:ILE:HD13	1:C:134:LEU:CD2	2.42	0.47
3:F:228:ILE:O	3:F:232:PRO:HG3	2.14	0.47
3:E:220:ALA:HB1	3:E:225:MET:O	2.14	0.47
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.49	0.47
1:A:265:THR:N	1:A:266:PRO:HD2	2.29	0.47
1:A:303:THR:HG22	9:A:1547:HOH:O	2.14	0.47
3:H:68:GLU:N	3:H:68:GLU:OE1	2.46	0.47
1:A:210:ARG:CD	1:A:263:GLU:OE2	2.59	0.47
3:E:20:GLN:O	3:E:23:VAL:HG22	2.14	0.47
3:E:218:GLN:OE1	3:E:218:GLN:N	2.47	0.47
3:F:130:VAL:HG23	3:F:130:VAL:O	2.13	0.47
3:F:58:MET:HG2	3:F:88:SER:O	2.14	0.47
3:E:166:LYS:HG2	3:E:258:PRO:HG3	1.97	0.47
1:A:442:HIS:CE1	7:A:1496:CFM:S1B	3.07	0.47
2:B:225:ASN:HB3	2:B:254:LEU:HD11	1.96	0.47
1:C:462:ASP:HA	1:C:465:MET:HG2	1.97	0.47
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.97	0.47
1:C:203:ARG:HG3	1:C:204:ASP:N	2.30	0.47
3:F:103:ILE:HG12	3:F:137:MET:HG2	1.95	0.47
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.43	0.47
3:F:183:ILE:HG12	3:F:208:ILE:HG22	1.97	0.47
2:D:67:ALA:H	2:D:396:HIS:HD2	1.63	0.47
2:D:74:GLY:HA3	2:D:193:HIS:O	2.15	0.47
1:A:47:ILE:HD12	1:A:50:LYS:HG3	1.97	0.47
2:D:373:PRO:O	2:D:377:MET:HB2	2.15	0.47
9:A:1624:HOH:O	2:B:119:THR:HG23	2.15	0.47
2:D:158:ILE:HG22	3:G:97:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:236:ASN:HD21	2:B:484:THR:HB	1.79	0.46
2:D:9:LYS:HB3	2:D:13:PRO:HD2	1.96	0.46
1:C:429:PHE:O	1:C:433:LYS:HD3	2.14	0.46
3:H:10:LYS:CE	3:H:11:GLY:H	2.29	0.46
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.97	0.46
3:H:130:VAL:HG23	3:H:130:VAL:O	2.15	0.46
3:H:119:LEU:CD1	3:H:119:LEU:N	2.78	0.46
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.97	0.46
1:C:198:ALA:O	1:C:202:VAL:HG23	2.15	0.46
3:G:261:MET:HG2	3:H:46:ARG:CZ	2.45	0.46
1:A:298:ASN:HD21	1:A:300:PHE:HB2	1.80	0.46
1:C:66:GLY:O	1:C:70:VAL:HG22	2.14	0.46
2:D:411:ALA:HA	2:D:417:LYS:NZ	2.30	0.46
3:F:33:VAL:HG12	3:F:34:MET:N	2.29	0.46
3:F:26:LEU:HD13	3:F:244:ALA:HB1	1.98	0.46
3:H:126:VAL:CG2	3:H:138:PRO:HG2	2.45	0.46
2:B:93:GLN:HG2	9:B:1547:HOH:O	2.15	0.46
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.97	0.46
1:A:274:HIS:HE1	1:A:299:PHE:H	1.62	0.46
1:A:151:GLN:HG3	1:A:183:CYS:SG	2.56	0.46
3:H:245:ARG:HD2	9:H:321:HOH:O	2.13	0.46
1:A:225:ILE:HD12	1:A:252:GLN:HG2	1.97	0.46
1:C:165:SER:O	1:C:169:VAL:HG22	2.15	0.46
1:A:113:ASN:ND2	9:A:1527:HOH:O	2.43	0.46
3:G:41:LYS:NZ	3:H:41:LYS:NZ	2.63	0.46
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.97	0.46
1:A:449:PRO:O	1:A:450:TYR:HD2	1.99	0.46
1:A:103:THR:H	1:A:107:ASN:ND2	2.11	0.46
2:D:103:PHE:HB3	2:D:111:VAL:HG11	1.98	0.46
3:H:68:GLU:H	3:H:68:GLU:CD	2.18	0.46
3:E:205:THR:HG23	3:E:206:GLN:N	2.31	0.46
3:E:261:MET:HG2	3:F:46:ARG:CZ	2.46	0.46
2:B:324:TRP:CZ3	2:B:378:GLY:HA2	2.51	0.46
1:A:62:CYS:O	1:A:191:GLN:HA	2.16	0.46
2:D:43:VAL:O	2:D:47:THR:HG23	2.16	0.46
3:F:137:MET:N	3:F:138:PRO:CD	2.79	0.46
1:C:359:ARG:HH11	1:C:442:HIS:HA	1.81	0.46
9:B:1500:HOH:O	1:C:433:LYS:HE2	2.16	0.46
3:F:67:VAL:HG12	3:F:108:PHE:CD1	2.51	0.46
3:G:238:ASP:HA	3:G:241:ARG:HD2	1.98	0.45
3:E:145:GLN:CA	3:E:145:GLN:HE21	2.29	0.45
3:H:67:VAL:HG21	3:H:104:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:GLU:HG3	2:B:190:VAL:HG22	1.97	0.45
6:C:3494:HCA:H22	7:C:3496:CFM:S3B	2.55	0.45
3:G:70:LEU:HD23	3:G:71:GLU:N	2.31	0.45
2:D:119:THR:HG22	2:D:120:GLU:H	1.81	0.45
3:E:70:LEU:HB3	3:E:108:PHE:CE1	2.51	0.45
2:B:457:HIS:CD2	2:D:512:MET:HB3	2.50	0.45
3:G:80:TYR:O	3:G:83:VAL:HG23	2.17	0.45
3:H:19:THR:O	3:H:23:VAL:HG13	2.16	0.45
3:G:46:ARG:NH1	3:G:46:ARG:HG3	2.28	0.45
3:G:214:ASP:HB3	3:G:236:GLN:NE2	2.31	0.45
3:G:267:LEU:O	3:G:271:PHE:HD1	2.00	0.45
3:F:37:GLY:HA3	3:F:87:GLU:OE2	2.16	0.45
3:H:208:ILE:HG13	3:H:246:LYS:HB3	1.99	0.45
3:G:34:MET:HE1	3:G:115:TYR:CD1	2.52	0.45
3:H:71:GLU:OE1	3:H:71:GLU:HA	2.16	0.45
3:G:178:ARG:CB	3:G:253:LEU:HB3	2.47	0.45
3:E:126:VAL:HG12	3:E:128:GLY:N	2.32	0.45
3:F:165:SER:O	3:F:169:VAL:HG23	2.16	0.45
3:F:147:ILE:O	3:F:179:LEU:HD23	2.16	0.45
1:A:6:ARG:CB	1:A:7:GLU:OE1	2.65	0.45
3:H:33:VAL:HG12	3:H:34:MET:N	2.32	0.45
3:G:199:LEU:O	3:G:203:LEU:HD13	2.16	0.45
2:B:71:GLN:O	2:B:196:GLY:HA3	2.17	0.45
3:H:57:ILE:HD11	3:H:86:VAL:CG1	2.46	0.45
1:A:74:PRO:HB2	1:A:254:SER:HB3	1.98	0.45
3:E:20:GLN:HA	3:E:23:VAL:HG22	1.99	0.45
2:B:103:PHE:HB3	2:B:111:VAL:HG11	1.99	0.45
2:B:406:VAL:HA	2:B:409:ILE:HD12	1.98	0.45
3:F:139:ILE:HG22	3:F:147:ILE:HD11	1.98	0.44
3:F:18:THR:HG21	3:F:185:ASN:OD1	2.17	0.44
3:E:150:VAL:HA	3:E:183:ILE:O	2.17	0.44
3:G:41:LYS:NZ	3:G:129:ASP:H	2.15	0.44
6:A:1494:HCA:H22	7:A:1496:CFM:S3B	2.57	0.44
3:H:84:LYS:NZ	3:H:117:ASP:OD2	2.45	0.44
3:G:72:LEU:O	3:G:75:VAL:HG12	2.18	0.44
2:D:119:THR:CG2	2:D:120:GLU:H	2.30	0.44
3:H:70:LEU:HB3	3:H:108:PHE:CE1	2.53	0.44
1:A:225:ILE:HG13	1:A:249:CYS:SG	2.57	0.44
3:G:9:GLY:HA3	3:G:150:VAL:HG22	1.99	0.44
2:D:381:LYS:O	2:D:385:GLU:HG3	2.17	0.44
2:D:260:VAL:HG22	9:D:3516:HOH:O	2.17	0.44
3:F:256:PRO:O	3:F:258:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:103:ILE:HG12	3:H:137:MET:CG	2.48	0.44
1:C:325:GLU:HA	1:C:328:ILE:HG23	1.94	0.44
3:F:253:LEU:HD22	3:F:253:LEU:N	2.32	0.44
1:C:100:TYR:CE2	1:C:110:VAL:HB	2.53	0.44
3:F:261:MET:SD	3:F:264:LEU:HD23	2.58	0.44
3:H:23:VAL:HG21	3:H:35:ILE:CD1	2.48	0.44
3:G:212:PRO:HG2	3:G:236:GLN:OE1	2.17	0.44
3:G:209:HIS:CG	3:G:210:PHE:N	2.86	0.44
3:E:144:ALA:O	3:E:177:VAL:HG23	2.17	0.44
3:H:75:VAL:HG22	9:H:293:HOH:O	2.17	0.44
3:F:146:GLU:HG2	3:F:253:LEU:CD1	2.47	0.44
1:C:138:VAL:HG12	2:D:62:LEU:HD22	1.98	0.44
3:E:88:SER:HB2	3:E:105:ALA:CB	2.48	0.44
3:F:8:TYR:O	3:F:149:ILE:HA	2.17	0.44
3:F:154:GLU:O	3:F:158:MET:HG3	2.18	0.44
1:A:378:GLY:HA3	1:A:401:TYR:CD2	2.53	0.44
3:H:10:LYS:HA	3:H:10:LYS:CE	2.46	0.44
3:F:164:ILE:O	3:F:168:ILE:HG13	2.18	0.44
3:E:145:GLN:HG2	9:E:5326:HOH:O	2.18	0.44
2:D:234:LEU:HD23	2:D:480:HIS:HD2	1.83	0.44
3:H:8:TYR:O	3:H:149:ILE:HA	2.17	0.43
1:C:68:LYS:CB	1:C:151:GLN:HG2	2.47	0.43
2:D:376:VAL:HG13	2:D:402:TRP:HZ2	1.83	0.43
3:E:88:SER:HB2	3:E:105:ALA:HB2	2.00	0.43
3:G:141:GLU:O	3:G:143:LYS:HG2	2.17	0.43
2:D:151:THR:CG2	2:D:162:LEU:HD21	2.48	0.43
3:G:265:GLU:O	3:G:269:MET:HG3	2.18	0.43
2:B:369:LEU:HD13	2:B:379:LEU:HD12	2.00	0.43
2:B:502:LEU:HD11	2:D:477:HIS:CD2	2.53	0.43
2:D:100:ARG:HA	2:D:111:VAL:HG21	1.99	0.43
3:H:186:SER:HA	3:H:192:GLU:OE1	2.18	0.43
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.47	0.43
1:C:442:HIS:HE1	7:C:3496:CFM:S1B	2.41	0.43
3:G:70:LEU:HD23	3:G:71:GLU:H	1.82	0.43
1:A:192:SER:OG	1:A:383:HIS:HE1	2.01	0.43
3:H:147:ILE:HG21	3:H:168:ILE:HD11	2.01	0.43
3:G:182:LEU:O	3:G:208:ILE:HG22	2.18	0.43
2:D:124:VAL:O	3:G:91:PRO:HB3	2.17	0.43
3:F:77:LYS:HZ3	3:F:77:LYS:HB3	1.83	0.43
1:C:355:ILE:HG22	1:C:356:GLY:H	1.84	0.43
3:F:245:ARG:HH11	3:F:245:ARG:HG2	1.83	0.43
3:E:137:MET:N	3:E:138:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:4:GLN:HB2	3:H:144:ALA:HA	2.00	0.43
3:F:177:VAL:O	3:F:177:VAL:HG13	2.18	0.43
2:B:473:ILE:CD1	2:B:479:LEU:HD23	2.48	0.43
3:E:261:MET:O	3:E:265:GLU:HG3	2.18	0.43
1:A:82:SER:HB2	1:A:115:THR:HG22	1.99	0.43
1:A:39:VAL:O	1:A:41:GLN:N	2.51	0.43
2:D:96:VAL:HA	2:D:99:PHE:CD2	2.53	0.43
3:H:183:ILE:HD13	3:H:243:LEU:HD11	2.00	0.43
2:D:28:ARG:HA	2:D:32:GLU:HB2	2.00	0.43
1:A:475:LEU:HD22	2:D:352:VAL:HG11	2.00	0.43
3:G:163:ASN:HD22	3:G:163:ASN:HA	1.64	0.43
3:F:179:LEU:CD2	3:F:181:GLY:H	2.29	0.43
3:G:4:GLN:CB	3:G:144:ALA:HA	2.48	0.43
1:C:477:ALA:HA	1:C:478:PRO:HD2	1.89	0.43
3:F:179:LEU:HD22	3:F:181:GLY:N	2.33	0.43
2:B:96:VAL:O	2:B:100:ARG:HG3	2.19	0.43
2:B:376:VAL:HG13	2:B:402:TRP:HZ2	1.84	0.43
1:A:462:ASP:HA	1:A:465:MET:HG2	2.01	0.43
1:A:124:VAL:O	3:F:91:PRO:HB3	2.19	0.43
2:B:310:LYS:HE2	9:B:1755:HOH:O	2.19	0.43
3:E:228:ILE:O	3:E:232:PRO:HG3	2.19	0.42
3:G:259:ILE:HD11	3:G:264:LEU:HD13	2.01	0.42
3:E:182:LEU:HD22	3:E:200:ALA:HB2	2.00	0.42
2:D:509:THR:O	2:D:516:ASP:HA	2.19	0.42
3:E:189:THR:HG22	3:F:213:ARG:HH22	1.84	0.42
1:C:82:SER:HB3	1:C:153:GLU:OE1	2.19	0.42
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.84	0.42
3:E:162:ASN:ND2	3:E:259:ILE:HG12	2.35	0.42
3:H:162:ASN:HD21	3:H:258:PRO:HA	1.83	0.42
1:A:274:HIS:HD2	9:A:1639:HOH:O	2.02	0.42
2:D:523:ARG:HD2	9:D:3587:HOH:O	2.18	0.42
2:B:206:ARG:HA	2:B:304:PHE:CZ	2.54	0.42
3:H:49:LEU:HD13	3:H:85:CYS:SG	2.59	0.42
3:H:46:ARG:HG3	3:H:46:ARG:NH1	2.33	0.42
2:D:416:GLY:C	2:D:417:LYS:HE2	2.40	0.42
3:H:10:LYS:O	3:H:13:ILE:HG12	2.20	0.42
3:G:43:ASP:OD1	3:G:46:ARG:HB2	2.20	0.42
2:D:119:THR:CG2	2:D:120:GLU:N	2.82	0.42
2:B:198:ASP:HB2	2:B:297:HIS:O	2.20	0.42
1:A:203:ARG:HG3	1:A:204:ASP:N	2.35	0.42
3:H:106:ILE:HB	3:H:137:MET:CE	2.50	0.42
3:F:41:LYS:HD3	3:F:41:LYS:N	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:3:ARG:O	3:F:121:PHE:HA	2.19	0.42
2:D:479:LEU:HB2	9:D:3510:HOH:O	2.18	0.42
2:B:348:ARG:HD3	1:C:479:TRP:CH2	2.54	0.42
3:H:60:MET:HE2	3:H:74:ASP:HB3	2.01	0.42
3:G:20:GLN:HA	3:G:23:VAL:HG22	2.00	0.42
3:G:21:ASN:N	3:G:21:ASN:ND2	2.67	0.42
2:B:146:MET:HG3	2:B:180:PRO:HB2	2.01	0.42
3:H:183:ILE:HG12	3:H:208:ILE:CG2	2.50	0.42
3:H:165:SER:O	3:H:169:VAL:HG23	2.19	0.42
3:F:56:THR:HG23	3:F:59:GLU:OE2	2.20	0.42
3:G:129:ASP:HB2	3:H:41:LYS:NZ	2.24	0.42
1:C:36:ASP:O	1:C:39:VAL:CG1	2.67	0.42
1:A:115:THR:HB	1:A:117:ASP:H	1.84	0.42
3:H:231:ASP:O	3:H:231:ASP:CG	2.59	0.42
3:G:205:THR:CG2	3:G:206:GLN:N	2.65	0.42
3:F:208:ILE:O	3:F:246:LYS:HD3	2.20	0.42
3:F:46:ARG:HH11	3:F:46:ARG:HG3	1.85	0.42
3:E:152:SER:O	3:E:196:ILE:HD11	2.19	0.42
3:H:236:GLN:O	3:H:239:GLU:HB2	2.19	0.42
2:B:509:THR:HG21	2:B:518:ASN:HD22	1.83	0.42
1:C:282:ILE:O	1:C:286:MET:HG3	2.19	0.42
2:B:479:LEU:HB2	9:B:1507:HOH:O	2.20	0.42
3:E:110:GLU:HG3	3:E:143:LYS:HZ3	1.85	0.42
3:G:73:GLU:H	3:G:73:GLU:CD	2.24	0.42
2:D:192:SER:OG	2:D:194:VAL:HG22	2.20	0.42
3:H:8:TYR:CB	3:H:164:ILE:HD13	2.46	0.41
2:B:104:ASN:OD1	2:B:111:VAL:HG22	2.21	0.41
2:B:348:ARG:O	2:B:352:VAL:HG23	2.20	0.41
2:B:522:VAL:HG22	9:B:1630:HOH:O	2.20	0.41
1:C:145:ASN:HD22	1:C:147:GLY:H	1.67	0.41
2:B:322:LEU:HD23	1:C:474:LYS:HD3	2.02	0.41
2:D:369:LEU:HD12	2:D:376:VAL:HG23	2.01	0.41
1:C:59:ILE:HD12	1:C:354:TYR:CE2	2.55	0.41
3:H:205:THR:OG1	3:H:206:GLN:N	2.50	0.41
3:G:20:GLN:OE1	3:G:47:LEU:HB2	2.20	0.41
1:A:68:LYS:CB	1:A:151:GLN:HG2	2.37	0.41
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.61	0.41
3:E:219:ARG:HD2	9:E:5334:HOH:O	2.19	0.41
1:A:186:PHE:HB3	2:B:154:MET:HE2	2.02	0.41
1:A:96:ARG:NH2	7:A:1496:CFM:S5	2.93	0.41
3:H:76:LEU:HD23	3:H:86:VAL:CG2	2.44	0.41
1:C:159:ILE:CG1	3:H:97:CYS:HB2	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:103:ILE:HA	3:H:137:MET:CE	2.49	0.41
2:D:376:VAL:HG13	2:D:402:TRP:CZ2	2.55	0.41
2:B:247:MET:HG2	2:B:341:PRO:CD	2.50	0.41
3:G:10:LYS:HE2	3:H:11:GLY:C	2.40	0.41
3:H:106:ILE:HB	3:H:137:MET:HE3	2.02	0.41
3:E:225:MET:CE	3:E:229:GLU:HG2	2.49	0.41
2:D:10:ALA:O	2:D:14:LEU:HB2	2.20	0.41
2:D:39:LYS:HA	2:D:39:LYS:HD2	1.84	0.41
2:D:411:ALA:HA	2:D:417:LYS:HZ1	1.84	0.41
1:C:357:GLY:HA2	1:C:379:TYR:CD2	2.54	0.41
3:H:153:GLY:HA3	3:H:192:GLU:HG3	2.03	0.41
1:A:39:VAL:HG21	1:A:391:MET:CE	2.50	0.41
1:A:159:ILE:HD11	3:F:97:CYS:CB	2.49	0.41
3:F:141:GLU:O	3:F:142:ASN:HB2	2.21	0.41
1:C:220:PRO:O	1:C:316:PHE:CE2	2.67	0.41
3:G:10:LYS:NZ	3:H:12:GLY:HA2	2.36	0.41
3:G:220:ALA:HB1	3:G:225:MET:O	2.21	0.41
3:H:208:ILE:CG1	3:H:246:LYS:HB3	2.51	0.41
3:F:56:THR:OG1	3:F:59:GLU:HG2	2.21	0.41
1:C:53:GLN:HA	1:C:54:PRO:HD2	1.91	0.41
1:C:5:SER:HA	1:C:8:GLU:HB3	2.03	0.41
3:G:228:ILE:O	3:G:232:PRO:HG3	2.20	0.41
3:F:19:THR:O	3:F:23:VAL:HG13	2.20	0.41
3:F:23:VAL:CG2	3:F:35:ILE:HD11	2.24	0.41
3:E:23:VAL:HG23	3:E:24:ALA:N	2.36	0.41
3:F:162:ASN:HD21	3:F:258:PRO:CA	2.26	0.41
3:H:10:LYS:HE2	3:H:11:GLY:N	2.32	0.41
3:F:225:MET:CE	3:F:229:GLU:HG2	2.51	0.41
3:F:8:TYR:HB3	3:F:164:ILE:HD13	2.02	0.41
3:H:60:MET:HE3	3:H:74:ASP:HB3	2.02	0.41
2:B:402:TRP:CZ2	2:B:406:VAL:HG21	2.56	0.41
1:A:298:ASN:ND2	1:A:300:PHE:H	2.19	0.41
3:G:211:VAL:HA	3:G:212:PRO:HD2	1.94	0.41
3:F:60:MET:HB3	3:F:70:LEU:HD21	2.03	0.41
1:C:9:VAL:HG23	1:C:34:VAL:HG11	2.03	0.41
1:A:355:ILE:CD1	1:A:359:ARG:HB2	2.51	0.41
3:E:26:LEU:CD1	3:E:244:ALA:HB1	2.50	0.41
3:H:68:GLU:N	3:H:68:GLU:CD	2.75	0.41
2:D:377:MET:HG3	2:D:406:VAL:HG22	2.02	0.41
3:G:13:ILE:CD1	3:G:151:CYS:HA	2.51	0.41
3:E:11:GLY:C	3:E:13:ILE:H	2.24	0.41
3:H:10:LYS:HE2	3:H:10:LYS:CA	2.49	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:208:ILE:HD11	3:E:246:LYS:HB3	2.02	0.40
1:C:332:LYS:N	1:C:333:PRO:HD2	2.36	0.40
3:H:20:GLN:OE1	3:H:47:LEU:HB2	2.21	0.40
2:D:449:LYS:HE3	2:D:449:LYS:HB2	1.95	0.40
3:G:194:GLU:HB3	3:G:271:PHE:HE2	1.86	0.40
2:B:497:LEU:O	2:B:501:ILE:HG13	2.22	0.40
3:G:261:MET:CG	3:H:46:ARG:NH2	2.84	0.40
3:E:23:VAL:O	3:E:26:LEU:HB2	2.22	0.40
3:F:261:MET:O	3:F:265:GLU:HG3	2.21	0.40
3:G:57:ILE:HG23	3:G:70:LEU:CD1	2.51	0.40
1:A:457:ALA:CB	2:B:3:GLN:HG2	2.51	0.40
2:D:445:ASN:HB2	2:D:472:PRO:O	2.21	0.40
3:G:185:ASN:O	3:G:186:SER:C	2.59	0.40
1:A:474:LYS:O	2:D:348:ARG:NH1	2.55	0.40
3:E:187:ARG:O	3:E:188:ASN:HB3	2.20	0.40
3:G:72:LEU:HB2	3:G:112:GLU:CG	2.44	0.40
2:D:373:PRO:HG2	9:D:3554:HOH:O	2.21	0.40
3:F:193:ASP:O	3:F:197:ILE:HG13	2.22	0.40
2:D:331:LYS:HD2	2:D:331:LYS:HA	1.93	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	474/492 (96%)	443 (94%)	28 (6%)	3 (1%)	33	32
1	C	474/492 (96%)	441 (93%)	29 (6%)	4 (1%)	27	24
2	B	520/523 (99%)	502 (96%)	17 (3%)	1 (0%)	56	62
2	D	520/523 (99%)	507 (98%)	11 (2%)	2 (0%)	43	45
3	E	251/289 (87%)	234 (93%)	16 (6%)	1 (0%)	43	45
3	F	254/289 (88%)	240 (94%)	12 (5%)	2 (1%)	27	24
3	G	249/289 (86%)	231 (93%)	16 (6%)	2 (1%)	27	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	256/289 (89%)	244 (95%)	10 (4%)	2 (1%)	27	24
All	All	2998/3186 (94%)	2842 (95%)	139 (5%)	17 (1%)	33	32

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	THR
3	F	118	ASP
1	A	40	THR
1	C	396	ASP
3	G	44	SER
3	H	11	GLY
1	A	396	ASP
2	B	255	SER
1	C	254	SER
2	D	117	SER
3	F	14	GLY
1	A	117	ASP
2	D	255	SER
1	C	87	GLY
3	H	12	GLY
3	G	130	VAL
3	E	12	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	405/415 (98%)	375 (93%)	30 (7%)	20	19
1	C	405/415 (98%)	379 (94%)	26 (6%)	25	26
2	B	454/455 (100%)	429 (94%)	25 (6%)	30	34
2	D	454/455 (100%)	427 (94%)	27 (6%)	28	30
3	E	206/233 (88%)	186 (90%)	20 (10%)	12	10
3	F	205/233 (88%)	191 (93%)	14 (7%)	22	23
3	G	204/233 (88%)	194 (95%)	10 (5%)	35	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	209/233 (90%)	198 (95%)	11 (5%)	32	36
All	All	2542/2672 (95%)	2379 (94%)	163 (6%)	25	26

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	GLN
1	A	19	VAL
1	A	68	LYS
1	A	93	ARG
1	A	98	ASN
1	A	107	ASN
1	A	131	LEU
1	A	141	LEU
1	A	151	GLN
1	A	159	ILE
1	A	161	ASP
1	A	199	ASN
1	A	239	ARG
1	A	264	LEU
1	A	267	LYS
1	A	288	GLU
1	A	298	ASN
1	A	346	LEU
1	A	359	ARG
1	A	362	HIS
1	A	370	LEU
1	A	377	THR
1	A	383	HIS
1	A	404	VAL
1	A	415	ARG
1	A	427	GLU
1	A	445	ASP
1	A	474	LYS
1	A	475	LEU
2	B	13	PRO
2	B	14	LEU
2	B	24	LEU
2	B	28	ARG
2	B	38	ASP
2	B	55	LEU

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Mol	Chain	Res	Type
2	B	154	MET
2	B	172	GLU
2	B	177	ASP
2	B	210	LEU
2	B	234	LEU
2	B	258	GLU
2	B	260	VAL
2	B	261	LEU
2	B	281	MET
2	B	315	LYS
2	B	369	LEU
2	B	379	LEU
2	B	383	LEU
2	B	386	LEU
2	B	461	GLU
2	B	468	ARG
2	B	479	LEU
2	B	498	VAL
2	B	523	ARG
1	C	12	LEU
1	C	14	GLN
1	C	68	LYS
1	C	70	VAL
1	C	93	ARG
1	C	98	ASN
1	C	115	THR
1	C	131	LEU
1	C	151	GLN
1	C	212	GLU
1	C	239	ARG
1	C	264	LEU
1	C	267	LYS
1	C	277	ARG
1	C	298	ASN
1	C	328	ILE
1	C	346	LEU
1	C	358	LEU
1	C	360	PRO
1	C	362	HIS
1	C	401	TYR
1	C	415	ARG
1	C	427	GLU

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Mol	Chain	Res	Type
1	C	437	PRO
1	C	445	ASP
1	C	475	LEU
2	D	11	SER
2	D	13	PRO
2	D	14	LEU
2	D	24	LEU
2	D	38	ASP
2	D	55	LEU
2	D	153	CYS
2	D	154	MET
2	D	172	GLU
2	D	211	LYS
2	D	214	ASP
2	D	260	VAL
2	D	261	LEU
2	D	281	MET
2	D	316	LEU
2	D	369	LEU
2	D	379	LEU
2	D	383	LEU
2	D	384	LEU
2	D	386	LEU
2	D	456	LEU
2	D	461	GLU
2	D	468	ARG
2	D	473	ILE
2	D	484	THR
2	D	498	VAL
2	D	523	ARG
3	E	22	LEU
3	E	26	LEU
3	E	67	VAL
3	E	70	LEU
3	E	71	GLU
3	E	112	GLU
3	E	145	GLN
3	E	150	VAL
3	E	154	GLU
3	E	156	MET
3	E	163	ASN
3	E	179	LEU

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Mol	Chain	Res	Type
3	E	188	ASN
3	E	199	LEU
3	E	203	LEU
3	E	215	ASN
3	E	218	GLN
3	E	235	LYS
3	E	243	LEU
3	E	253	LEU
3	F	2	MET
3	F	22	LEU
3	F	26	LEU
3	F	41	LYS
3	F	71	GLU
3	F	112	GLU
3	F	145	GLN
3	F	154	GLU
3	F	162	ASN
3	F	163	ASN
3	F	179	LEU
3	F	182	LEU
3	F	218	GLN
3	F	243	LEU
3	G	2	MET
3	G	21	ASN
3	G	22	LEU
3	G	47	LEU
3	G	58	MET
3	G	70	LEU
3	G	75	VAL
3	G	145	GLN
3	G	154	GLU
3	G	235	LYS
3	H	2	MET
3	H	10	LYS
3	H	23	VAL
3	H	40	PRO
3	H	49	LEU
3	H	50	HIS
3	H	68	GLU
3	H	70	LEU
3	H	163	ASN
3	H	218	GLN

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Mol	Chain	Res	Type
3	H	243	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	113	ASN
1	A	145	ASN
1	A	151	GLN
1	A	230	ASN
1	A	271	ASN
1	A	274	HIS
1	A	285	HIS
1	A	298	ASN
1	A	362	HIS
1	A	383	HIS
2	B	3	GLN
2	B	130	ASN
2	B	136	GLN
2	B	168	ASN
2	B	185	HIS
2	B	396	HIS
2	B	457	HIS
2	B	518	ASN
2	B	519	HIS
1	C	107	ASN
1	C	113	ASN
1	C	145	ASN
1	C	230	ASN
1	C	271	ASN
1	C	298	ASN
1	C	383	HIS
1	C	476	GLN
2	D	3	GLN
2	D	104	ASN
2	D	130	ASN
2	D	163	ASN
2	D	168	ASN
2	D	396	HIS
2	D	518	ASN
2	D	519	HIS
3	E	142	ASN

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Mol	Chain	Res	Type
3	E	145	GLN
3	E	162	ASN
3	E	163	ASN
3	E	188	ASN
3	E	201	ASN
3	E	215	ASN
3	F	4	GLN
3	F	142	ASN
3	F	145	GLN
3	F	162	ASN
3	F	163	ASN
3	F	201	ASN
3	F	215	ASN
3	F	257	ASN
3	G	4	GLN
3	G	21	ASN
3	G	142	ASN
3	G	162	ASN
3	G	163	ASN
3	G	201	ASN
3	H	4	GLN
3	H	162	ASN
3	H	163	ASN
3	H	185	ASN
3	H	257	ASN

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 10 ligands modelled in this entry, 2 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	HCA	A	1494	-	13,13,13	2.42	4 (30%)	18,18,18	3.54	9 (50%)
7	CFM	A	1496	1	18,24,24	7.75	13 (72%)	0,45,45	0.00	-
8	CLF	B	1498	1,2	18,24,24	77.14	14 (77%)	0,57,57	0.00	-
6	HCA	C	3494	-	13,13,13	2.75	4 (30%)	18,18,18	3.96	11 (61%)
7	CFM	C	3496	1	18,24,24	7.51	16 (88%)	0,45,45	0.00	-
8	CLF	D	3498	1,2	18,24,24	76.44	14 (77%)	0,57,57	0.00	-
5	SF4	E	5290	3	12,12,12	3.53	10 (83%)	0,24,24	0.00	-
5	SF4	G	7290	3	12,12,12	1.00	0	0,24,24	0.00	-

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	HCA	A	1494	-	-	0/17/17/17	0/0/0/0
7	CFM	A	1496	1	-	0/0/84/84	0/0/8/8
8	CLF	B	1498	1,2	-	0/0/132/132	0/0/10/10
6	HCA	C	3494	-	-	0/17/17/17	0/0/0/0
7	CFM	C	3496	1	-	0/0/84/84	0/0/8/8
8	CLF	D	3498	1,2	-	0/0/132/132	0/0/10/10
5	SF4	E	5290	3	-	0/0/48/48	0/0/5/5
5	SF4	G	7290	3	-	0/0/48/48	0/0/5/5

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1498	CLF	S4A-FE2	234.13	3.90	2.33
8	D	3498	CLF	S4A-FE2	233.18	3.90	2.33
8	B	1498	CLF	S3A-FE1	227.44	3.86	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	3498	CLF	S3A-FE1	224.21	3.84	2.33
7	C	3496	CFM	S1A-FE1	-15.02	2.23	2.33
7	A	1496	CFM	S1B-FE5	-13.95	2.23	2.33
7	C	3496	CFM	S4B-FE7	-13.62	2.24	2.33
7	A	1496	CFM	S4A-FE3	-12.78	2.24	2.33
7	C	3496	CFM	S1B-FE6	-12.59	2.24	2.33
8	D	3498	CLF	S2A-FE3	-12.53	2.24	2.33
7	A	1496	CFM	S4A-FE1	-12.24	2.25	2.33
7	A	1496	CFM	S4B-FE7	-11.80	2.25	2.33
7	A	1496	CFM	S1A-FE4	-11.65	2.25	2.33
7	C	3496	CFM	S1B-FE5	-11.44	2.25	2.33
8	B	1498	CLF	S2A-FE1	-10.87	2.25	2.33
8	B	1498	CLF	S2A-FE3	-10.44	2.26	2.33
7	A	1496	CFM	S4B-FE5	-9.72	2.26	2.33
8	D	3498	CLF	S2A-FE1	-9.63	2.26	2.33
8	B	1498	CLF	S2A-FE2	-8.94	2.27	2.33
6	C	3494	HCA	O5-C7	7.99	1.49	1.22
8	D	3498	CLF	S2B-FE5	-7.79	2.28	2.33
8	D	3498	CLF	S2B-FE7	-7.66	2.28	2.33
8	B	1498	CLF	S3B-FE8	-7.37	2.28	2.33
8	B	1498	CLF	S2B-FE5	-7.37	2.28	2.33
7	A	1496	CFM	S2A-FE1	-7.18	2.28	2.33
7	A	1496	CFM	S1A-FE2	-7.01	2.28	2.33
7	A	1496	CFM	S1B-FE6	-6.98	2.28	2.33
5	E	5290	SF4	S4-FE3	-6.64	2.28	2.33
6	A	1494	HCA	O5-C7	6.62	1.45	1.22
7	C	3496	CFM	S4B-FE5	-6.49	2.28	2.33
8	B	1498	CLF	S3A-FE4	-6.39	2.29	2.33
7	C	3496	CFM	S1A-FE2	-6.33	2.29	2.33
8	D	3498	CLF	S2A-FE2	-6.11	2.29	2.33
7	C	3496	CFM	S3B-FE7	-5.95	2.29	2.33
5	E	5290	SF4	S2-FE3	-5.83	2.29	2.33
8	B	1498	CLF	S3B-FE7	-5.79	2.29	2.33
7	C	3496	CFM	S2A-FE2	-5.78	2.29	2.33
8	D	3498	CLF	S3B-FE8	-5.70	2.29	2.33
8	D	3498	CLF	S3A-FE4	-5.69	2.29	2.33
7	C	3496	CFM	MO1-S1B	5.67	2.37	2.31
7	C	3496	CFM	S2A-FE1	-5.60	2.29	2.33
7	C	3496	CFM	S1A-FE4	-5.39	2.29	2.33
7	C	3496	CFM	S4A-FE3	-5.19	2.29	2.33
8	B	1498	CLF	S4B-FE8	-5.19	2.29	2.33
8	D	3498	CLF	S3B-FE7	-5.13	2.29	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1496	CFM	MO1-S1B	4.86	2.37	2.31
5	E	5290	SF4	S3-FE2	-4.33	2.30	2.33
8	B	1498	CLF	S3A-FE3	-4.33	2.30	2.33
8	D	3498	CLF	S3B-FE6	-4.26	2.30	2.33
7	C	3496	CFM	S4A-FE1	-3.97	2.30	2.33
5	E	5290	SF4	S1-FE3	-3.55	2.30	2.33
6	C	3494	HCA	C3-C7	3.53	1.57	1.53
7	A	1496	CFM	MO1-S3B	3.40	2.35	2.31
5	E	5290	SF4	S2-FE1	3.37	2.35	2.33
7	C	3496	CFM	S4A-FE4	-3.32	2.31	2.33
7	A	1496	CFM	S2A-FE3	-3.27	2.31	2.33
6	A	1494	HCA	O6-C7	-3.09	1.18	1.30
6	C	3494	HCA	O1-C1	3.04	1.33	1.22
8	D	3498	CLF	S3A-FE3	-2.83	2.31	2.33
7	C	3496	CFM	S2A-FE3	-2.78	2.31	2.33
5	E	5290	SF4	S4-FE1	2.74	2.35	2.33
6	A	1494	HCA	C3-C7	2.72	1.56	1.53
8	B	1498	CLF	S4A-FE4	-2.66	2.31	2.33
6	A	1494	HCA	O1-C1	2.66	1.31	1.22
8	B	1498	CLF	S3B-FE6	-2.53	2.31	2.33
6	C	3494	HCA	O6-C7	-2.40	1.21	1.30
7	C	3496	CFM	S3B-FE6	2.35	2.34	2.33
5	E	5290	SF4	S1-FE4	2.35	2.34	2.33
5	E	5290	SF4	S4-FE2	-2.31	2.31	2.33
5	E	5290	SF4	S2-FE4	2.26	2.34	2.33
8	B	1498	CLF	S2B-FE6	-2.25	2.31	2.33
7	A	1496	CFM	S3B-FE7	-2.23	2.31	2.33
8	D	3498	CLF	S2B-FE6	-2.22	2.31	2.33
8	D	3498	CLF	S4A-FE4	-2.15	2.31	2.33
5	E	5290	SF4	S3-FE4	2.02	2.34	2.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3494	HCA	O7-C3-C2	-9.53	90.01	109.22
6	A	1494	HCA	O7-C3-C2	-9.19	90.70	109.22
6	A	1494	HCA	C3-C2-C1	6.95	130.60	113.77
6	C	3494	HCA	C3-C2-C1	6.88	130.45	113.77
6	C	3494	HCA	O7-C3-C4	-6.00	92.25	107.28
6	C	3494	HCA	C4-C3-C2	5.82	130.55	111.68
6	A	1494	HCA	C4-C3-C2	5.42	129.24	111.68
6	C	3494	HCA	O5-C7-C3	-5.36	114.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1494	HCA	O7-C3-C4	-4.14	96.90	107.28
6	A	1494	HCA	O6-C7-C3	4.05	118.79	112.89
6	C	3494	HCA	O7-C3-C7	3.40	113.85	108.95
6	C	3494	HCA	O6-C7-C3	3.14	117.46	112.89
6	C	3494	HCA	O2-C1-O1	-2.75	116.30	123.30
6	A	1494	HCA	O2-C1-O1	-2.57	116.75	123.30
6	A	1494	HCA	O5-C7-C3	-2.41	118.87	122.20
6	C	3494	HCA	O3-C6-C5	-2.29	115.14	123.03
6	A	1494	HCA	O3-C6-C5	-2.19	115.50	123.03
6	C	3494	HCA	C4-C3-C7	2.18	115.40	110.31
6	C	3494	HCA	O1-C1-C2	2.16	129.60	122.74
6	A	1494	HCA	O1-C1-C2	2.03	129.17	122.74

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.