Full wwPDB X-ray Structure Validation Report (i)

Jul 13, 2021 – 10:06 AM EDT

PDB ID	:	1N2C
Title	:	NITROGENASE COMPLEX FROM AZOTOBACTER VINELANDII STABILIZED BY ADP-TETRAFLUOROALUMINATE
Authors	:	Schindelin, H.; Kisker, C.; Rees, D.C.
Deposited on	:	1997-05-02
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

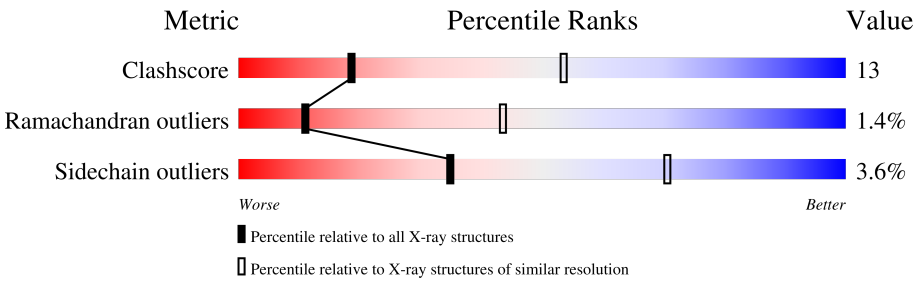
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	65% 30% • •
1	C	491	64% 31% • •
2	B	522	73% 26% •
2	D	522	70% 29% •
3	E	289	65% 28% • 5%
3	F	289	65% 27% • 5%
3	G	289	65% 28% • 5%
3	H	289	64% 28% • 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	A	496	-	-	X	-
5	CFM	C	496	-	-	X	-
7	CLF	B	525	-	-	X	-
7	CLF	D	525	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	478	3792	2411	647	710	24	0	0	0
1	C	478	3792	2411	647	710	24	0	0	0

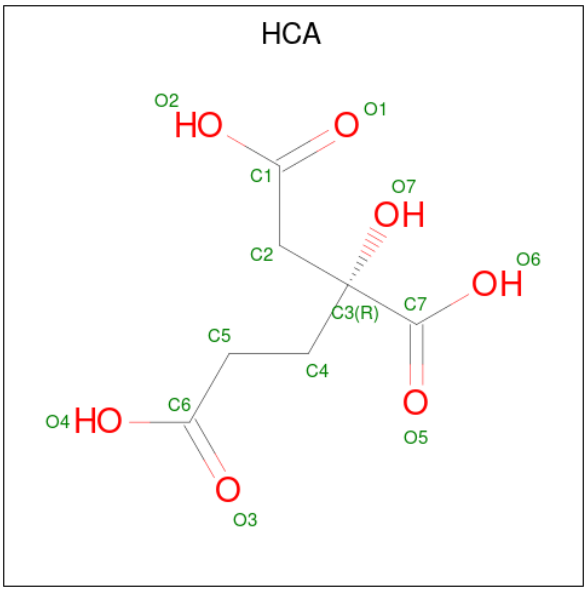
- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4170	2663	704	775	28	0	0	0
2	D	522	4170	2663	704	775	28	0	0	0

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

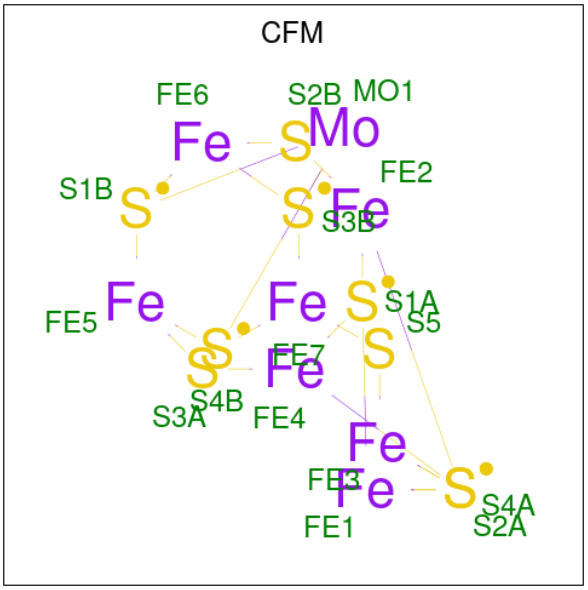
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	274	2065	1291	352	401	21	0	0	0
3	F	274	2065	1291	352	401	21	0	0	0
3	G	274	2065	1291	352	401	21	0	0	0
3	H	274	2065	1291	352	401	21	0	0	0

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



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

- Molecule 5 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).

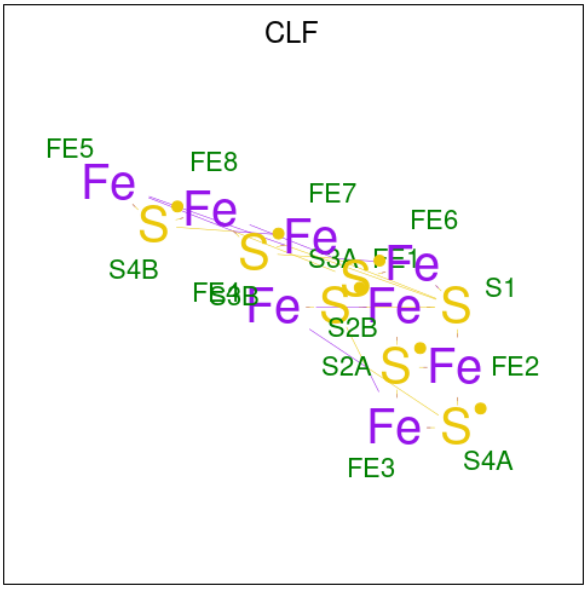


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Mo	S		
5	A	1	17	7	1	9	0	0
			Total	Fe	Mo	S		
5	C	1	17	7	1	9	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

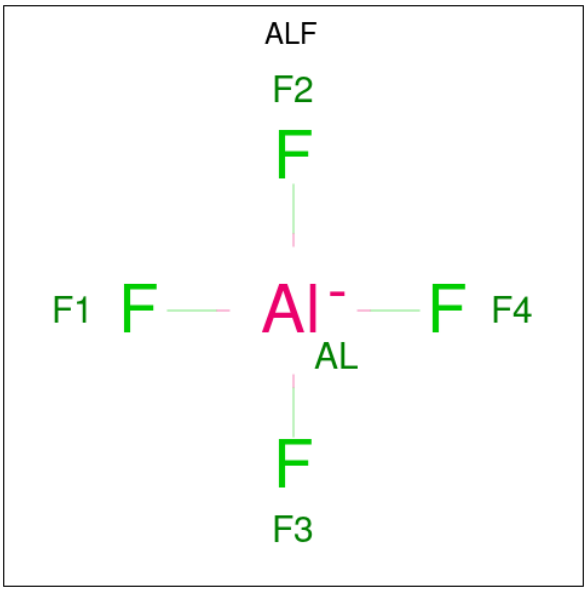


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 15 8 7	0	0
7	D	1	Total Fe S 15 8 7	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

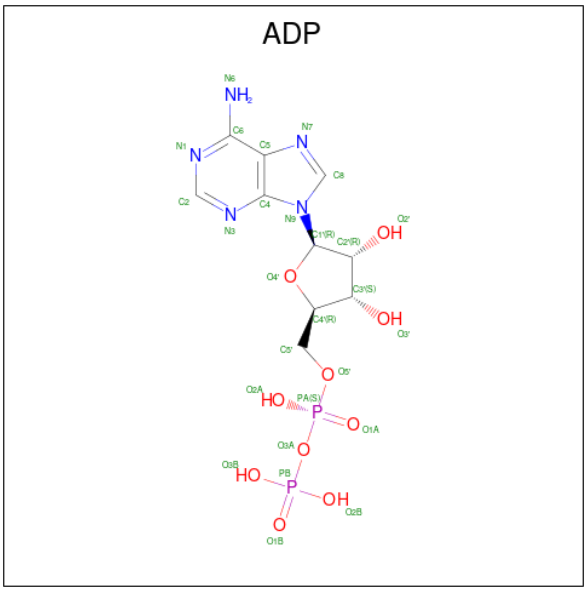
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Mg 1 1	0	0
8	F	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0

- Molecule 9 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



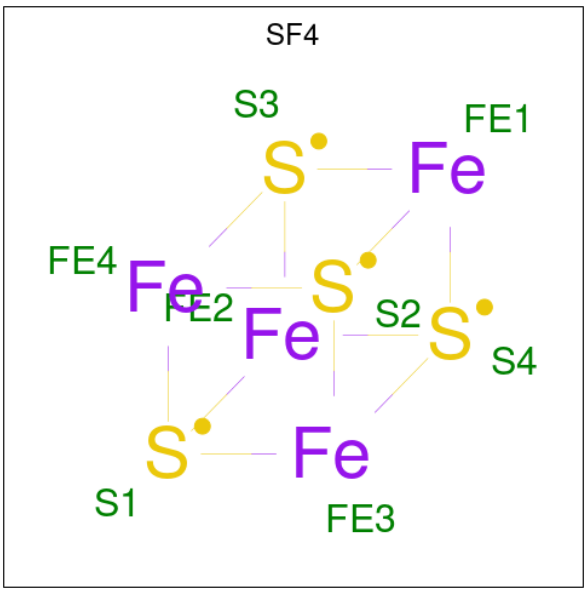
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
9	E	1	5	1	4	0	0
9	F	1	5	1	4	0	0
9	G	1	5	1	4	0	0
9	H	1	5	1	4	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	E	1	27	10	5	10	2	0	0
10	F	1	27	10	5	10	2	0	0
10	G	1	27	10	5	10	2	0	0
10	H	1	27	10	5	10	2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	F	1	8	4	4	0	0
11	G	1	8	4	4	0	0

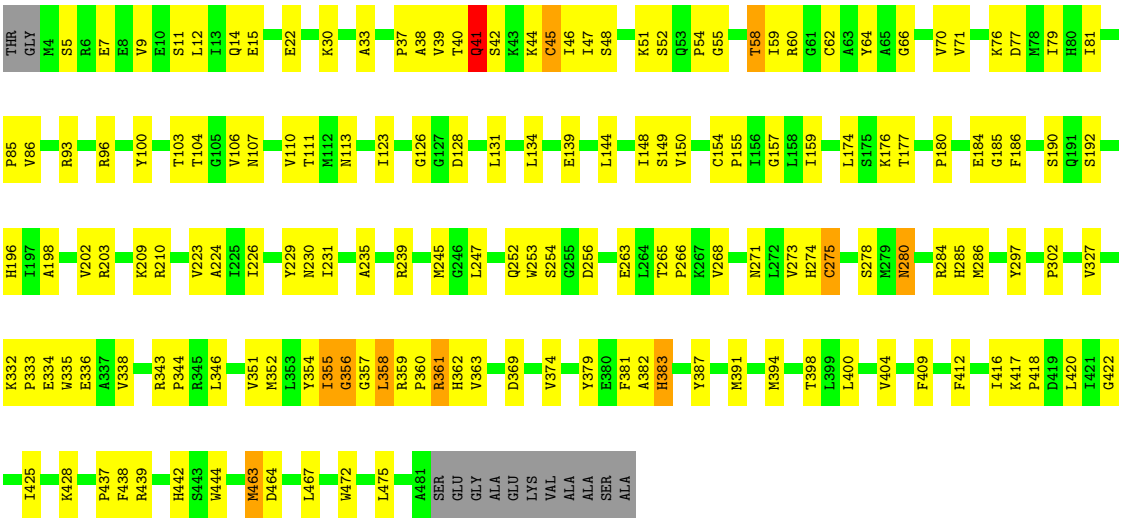
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

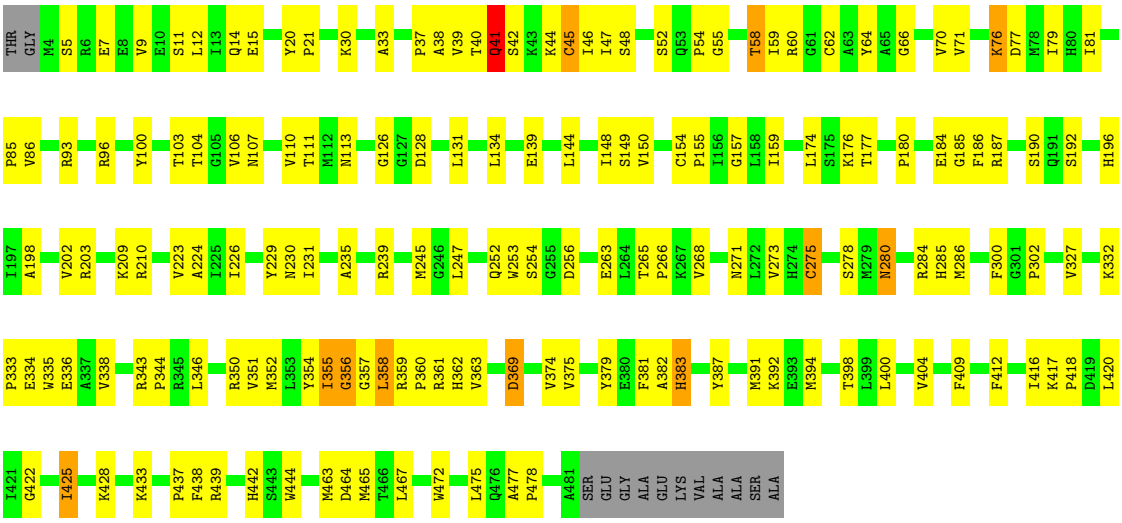
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN

Chain A:



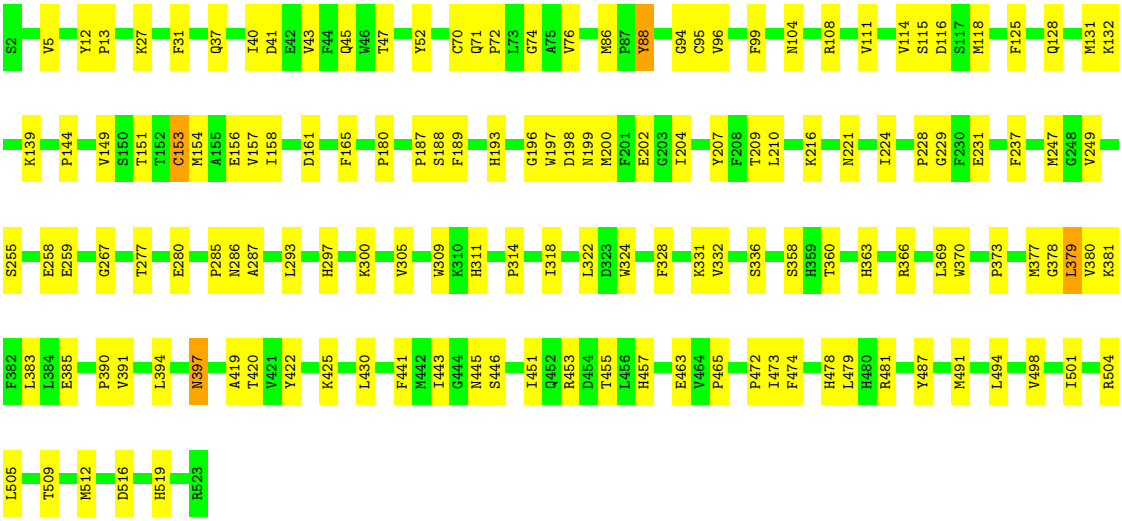
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN

Chain C:



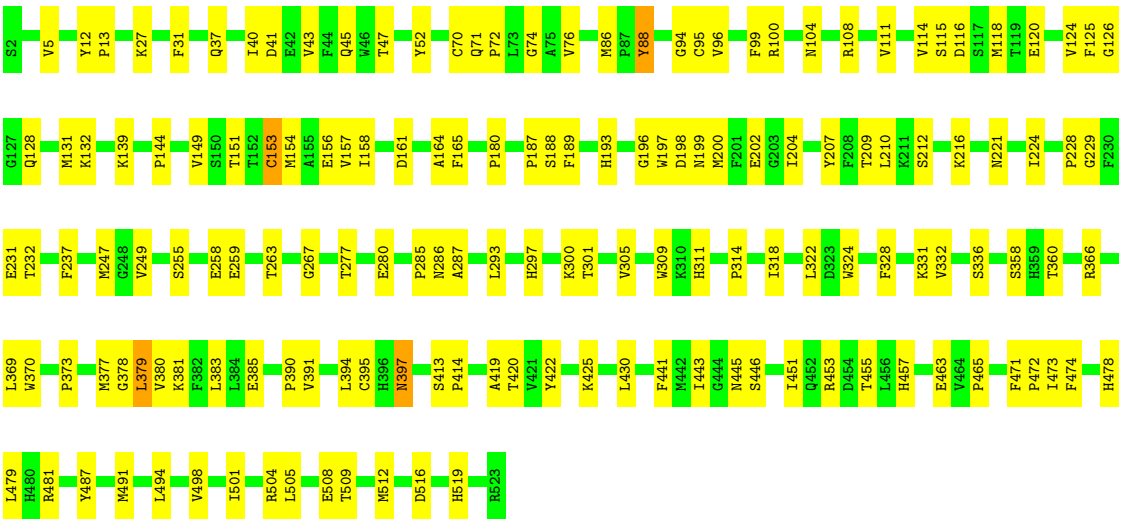
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN

Chain B: 73% 26% •



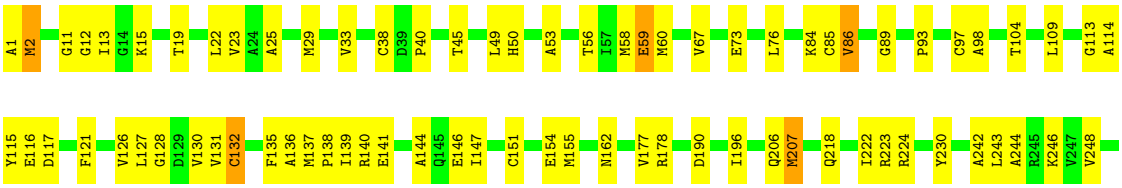
• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN

Chain D: 70% 29% •



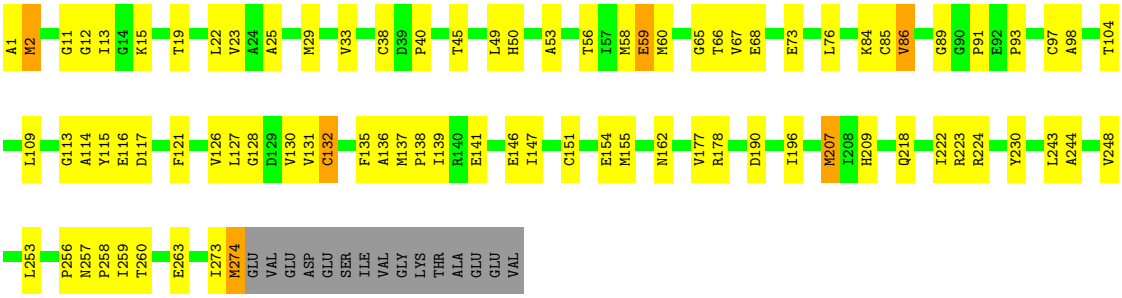
• Molecule 3: NITROGENASE IRON PROTEIN

Chain E: 65% 28% • 5%



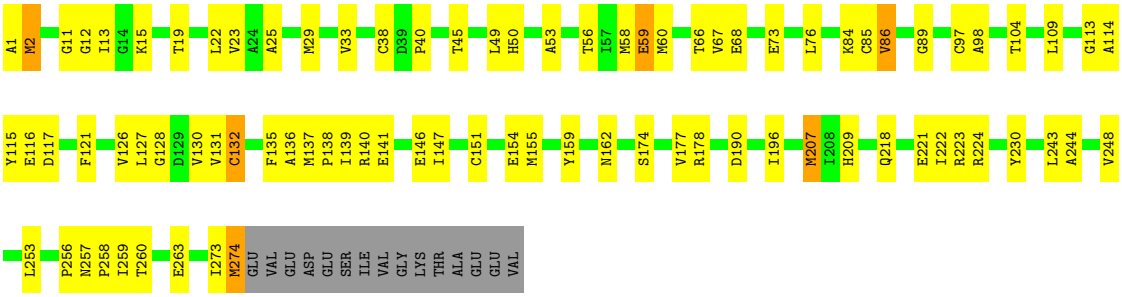
• Molecule 3: NITROGENASE IRON PROTEIN

Chain F:



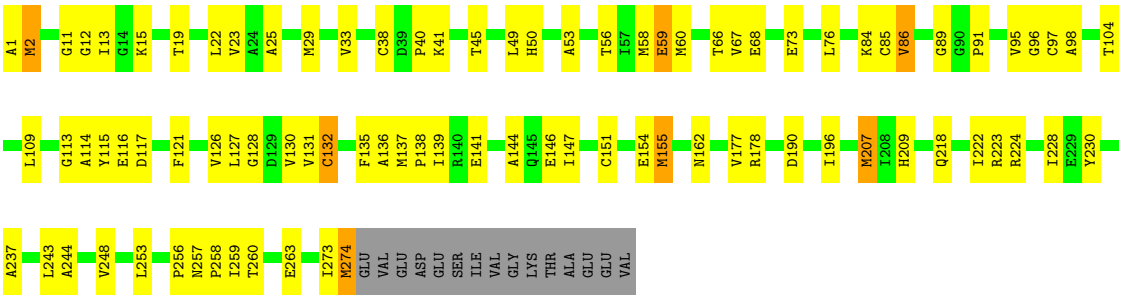
• Molecule 3: NITROGENASE IRON PROTEIN

Chain G:



• Molecule 3: NITROGENASE IRON PROTEIN

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	79.00Å 299.70Å 334.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	73.8 (50.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.208 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24426	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.32	0/3880	0.59	1/5233 (0.0%)
1	C	0.32	0/3880	0.59	1/5233 (0.0%)
2	B	0.32	0/4276	0.55	0/5782
2	D	0.32	0/4276	0.55	0/5782
3	E	0.31	0/2089	0.57	0/2815
3	F	0.30	0/2089	0.57	0/2815
3	G	0.31	0/2089	0.57	0/2815
3	H	0.30	0/2089	0.57	0/2815
All	All	0.32	0/24668	0.57	2/33290 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	275	CYS	CA-CB-SG	-6.21	102.83	114.00
1	A	275	CYS	CA-CB-SG	-6.00	103.20	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3792	0	3727	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3792	0	3727	127	0
2	B	4170	0	4076	107	0
2	D	4170	0	4076	115	0
3	E	2065	0	2077	55	0
3	F	2065	0	2077	58	0
3	G	2065	0	2077	58	0
3	H	2065	0	2077	58	0
4	A	14	0	6	1	0
4	C	14	0	6	1	0
5	A	17	0	0	6	0
5	C	17	0	0	7	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	15	0	0	4	0
7	D	15	0	0	4	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	E	5	0	0	0	0
9	F	5	0	0	0	0
9	G	5	0	0	0	0
9	H	5	0	0	0	0
10	E	27	0	12	2	0
10	F	27	0	12	2	0
10	G	27	0	12	2	0
10	H	27	0	12	2	0
11	F	8	0	0	0	0
11	G	8	0	0	0	0
All	All	24426	0	23974	637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (637) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ILE:HG22	3:F:97:CYS:HB2	1.48	0.93
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.62	0.81
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.62	0.80
2:B:125:PHE:HA	3:F:91:PRO:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:136:ALA:O	3:E:139:ILE:HG22	1.84	0.78
3:G:136:ALA:O	3:G:139:ILE:HG22	1.84	0.78
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.66	0.78
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.67	0.77
3:F:136:ALA:O	3:F:139:ILE:HG22	1.85	0.77
2:D:158:ILE:HG22	3:H:97:CYS:HB2	1.66	0.76
3:H:136:ALA:O	3:H:139:ILE:HG22	1.85	0.75
2:B:216:LYS:HG2	2:B:285:PRO:HB2	1.69	0.74
3:G:58:MET:HB2	3:G:89:GLY:HA3	1.70	0.74
1:A:226:ILE:HD11	1:A:273:VAL:HG22	1.69	0.74
3:F:58:MET:HB2	3:F:89:GLY:HA3	1.68	0.73
3:H:58:MET:HB2	3:H:89:GLY:HA3	1.69	0.73
1:C:39:VAL:HG11	1:C:44:LYS:HB2	1.71	0.73
2:D:216:LYS:HG2	2:D:285:PRO:HB2	1.69	0.73
2:D:128:GLN:HG2	2:D:132:LYS:HE3	1.71	0.73
2:B:128:GLN:HG2	2:B:132:LYS:HE3	1.71	0.72
3:G:131:VAL:HB	3:H:98:ALA:HB3	1.72	0.72
2:D:188:SER:HB3	7:D:525:CLF:S2B	2.29	0.72
1:A:39:VAL:HG11	1:A:44:LYS:HB2	1.71	0.72
1:C:226:ILE:HD11	1:C:273:VAL:HG22	1.71	0.72
2:D:125:PHE:HA	3:H:91:PRO:HB3	1.69	0.72
3:E:13:ILE:HG12	3:E:151:CYS:HA	1.71	0.71
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.54	0.71
3:G:13:ILE:HG12	3:G:151:CYS:HA	1.73	0.71
2:D:209:THR:HG21	2:D:309:TRP:HE1	1.55	0.71
1:A:239:ARG:HD2	1:A:252:GLN:HE21	1.56	0.70
3:E:58:MET:HB2	3:E:89:GLY:HA3	1.72	0.70
1:C:150:VAL:HG22	1:C:180:PRO:HA	1.73	0.70
3:H:13:ILE:HG12	3:H:151:CYS:HA	1.72	0.70
1:A:150:VAL:HG22	1:A:180:PRO:HA	1.73	0.70
3:E:76:LEU:HD13	3:E:86:VAL:HG22	1.73	0.70
1:C:239:ARG:HD2	1:C:252:GLN:HE21	1.56	0.70
3:H:76:LEU:HD13	3:H:86:VAL:HG22	1.74	0.69
3:F:13:ILE:HG12	3:F:151:CYS:HA	1.72	0.69
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.08	0.69
1:A:103:THR:HB	1:A:106:VAL:HG22	1.75	0.69
1:C:157:GLY:HA3	1:C:184:GLU:HG2	1.75	0.69
3:F:76:LEU:HD13	3:F:86:VAL:HG22	1.74	0.69
3:G:76:LEU:HD13	3:G:86:VAL:HG22	1.75	0.69
1:C:103:THR:HB	1:C:106:VAL:HG22	1.75	0.68
1:A:157:GLY:HA3	1:A:184:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:139:ILE:HG13	3:F:177:VAL:HG11	1.75	0.68
3:F:15:LYS:HG2	10:F:291:ADP:O2B	1.94	0.68
3:H:139:ILE:HG13	3:H:177:VAL:HG11	1.76	0.68
2:B:221:ASN:OD1	2:B:287:ALA:HA	1.94	0.67
1:C:192:SER:OG	1:C:383:HIS:HE1	1.78	0.67
1:A:192:SER:OG	1:A:383:HIS:HE1	1.78	0.67
1:C:96:ARG:NH2	5:C:496:CFM:S5	2.67	0.67
2:B:188:SER:HB3	7:B:525:CLF:S2B	2.34	0.67
2:D:221:ASN:OD1	2:D:287:ALA:HA	1.95	0.67
3:E:139:ILE:HG13	3:E:177:VAL:HG11	1.76	0.67
1:A:52:SER:HB3	1:A:58:THR:HG21	1.75	0.67
1:A:224:ALA:HB2	1:A:268:VAL:HG11	1.77	0.67
2:D:209:THR:HG21	2:D:309:TRP:NE1	2.09	0.66
1:C:224:ALA:HB2	1:C:268:VAL:HG11	1.77	0.66
3:G:139:ILE:HG13	3:G:177:VAL:HG11	1.76	0.66
3:H:15:LYS:HG2	10:H:291:ADP:O2B	1.95	0.66
3:E:40:PRO:HG3	3:E:98:ALA:HB1	1.78	0.66
3:H:45:THR:HG21	3:H:85:CYS:HB3	1.77	0.66
3:E:15:LYS:HG2	10:E:291:ADP:O2B	1.95	0.66
3:G:15:LYS:HG2	10:G:291:ADP:O2B	1.95	0.66
3:G:45:THR:HG21	3:G:85:CYS:HB3	1.77	0.66
1:C:52:SER:HB3	1:C:58:THR:HG21	1.77	0.66
2:D:12:TYR:HB3	2:D:13:PRO:HD3	1.78	0.65
2:D:314:PRO:HB3	2:D:331:LYS:HE2	1.78	0.65
3:F:40:PRO:HG3	3:F:98:ALA:HB1	1.79	0.65
1:A:96:ARG:NH2	5:A:496:CFM:S5	2.69	0.65
3:F:45:THR:HG21	3:F:85:CYS:HB3	1.77	0.65
3:E:131:VAL:HB	3:F:98:ALA:HB3	1.78	0.65
1:C:346:LEU:HD22	1:C:467:LEU:HD23	1.79	0.65
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.12	0.65
1:C:224:ALA:HB3	1:C:271:ASN:ND2	2.12	0.65
1:C:442:HIS:HE1	5:C:496:CFM:S1B	2.19	0.65
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.78	0.65
1:C:230:ASN:HA	1:C:235:ALA:H	1.62	0.64
2:D:509:THR:O	2:D:516:ASP:HA	1.98	0.64
2:B:12:TYR:HB3	2:B:13:PRO:HD3	1.79	0.64
1:A:442:HIS:HE1	5:A:496:CFM:S1B	2.20	0.64
3:G:40:PRO:HG3	3:G:98:ALA:HB1	1.78	0.64
1:A:346:LEU:HD22	1:A:467:LEU:HD23	1.79	0.63
3:H:40:PRO:HG3	3:H:98:ALA:HB1	1.79	0.63
2:B:509:THR:O	2:B:516:ASP:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:PRO:HB3	2:B:331:LYS:HE2	1.79	0.63
1:C:159:ILE:HG22	3:G:97:CYS:HB2	1.81	0.63
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.13	0.63
1:A:224:ALA:HB3	1:A:271:ASN:ND2	2.14	0.63
10:G:291:ADP:O3'	3:H:154:GLU:HB3	1.99	0.63
1:C:229:TYR:CE2	5:C:496:CFM:S2A	2.92	0.62
1:A:229:TYR:CE2	5:A:496:CFM:S2A	2.93	0.62
1:A:230:ASN:HA	1:A:235:ALA:H	1.63	0.62
2:B:216:LYS:HG3	2:B:286:ASN:OD1	2.00	0.62
2:D:139:LYS:HA	2:D:144:PRO:HD2	1.81	0.62
2:B:366:ARG:HE	2:B:391:VAL:HG11	1.64	0.61
3:E:98:ALA:HB3	3:F:131:VAL:HB	1.82	0.61
2:D:216:LYS:HG3	2:D:286:ASN:OD1	1.99	0.61
1:A:62:CYS:HB2	1:A:185:GLY:HA2	1.82	0.61
10:E:291:ADP:O3'	3:F:154:GLU:HB3	2.01	0.61
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.82	0.61
2:B:139:LYS:HA	2:B:144:PRO:HD2	1.82	0.61
2:D:366:ARG:HE	2:D:391:VAL:HG11	1.65	0.60
3:G:154:GLU:HB3	10:H:291:ADP:O3'	2.01	0.60
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.82	0.60
1:C:192:SER:HB2	1:C:381:PHE:HB2	1.83	0.60
1:A:192:SER:HB2	1:A:381:PHE:HB2	1.82	0.59
1:C:265:THR:O	1:C:268:VAL:HG22	2.02	0.59
3:G:244:ALA:O	3:G:248:VAL:HG23	2.03	0.59
1:A:265:THR:O	1:A:268:VAL:HG22	2.03	0.59
1:A:59:ILE:HD12	1:A:354:TYR:CE2	2.37	0.59
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.32	0.59
2:B:231:GLU:HB3	2:B:237:PHE:CZ	2.38	0.59
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.38	0.59
3:E:154:GLU:HB3	10:F:291:ADP:O3'	2.02	0.59
3:H:244:ALA:O	3:H:248:VAL:HG23	2.02	0.59
1:A:332:LYS:O	1:A:336:GLU:HB2	2.03	0.58
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.33	0.58
1:C:59:ILE:HD12	1:C:354:TYR:CE2	2.37	0.58
3:F:244:ALA:O	3:F:248:VAL:HG23	2.03	0.58
2:B:71:GLN:HE22	2:B:199:ASN:ND2	2.00	0.58
1:C:62:CYS:HB2	1:C:185:GLY:HA2	1.84	0.58
2:D:71:GLN:HE22	2:D:199:ASN:ND2	2.01	0.58
1:A:355:ILE:HG22	1:A:356:GLY:H	1.68	0.58
1:A:357:GLY:HA2	1:A:379:TYR:HD2	1.68	0.58
1:C:355:ILE:HG22	1:C:356:GLY:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:12:GLY:HA3	3:H:11:GLY:O	2.04	0.57
2:B:370:TRP:HA	2:B:394:LEU:O	2.05	0.57
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.69	0.57
1:A:106:VAL:HG21	2:B:40:ILE:HG23	1.86	0.57
1:A:256:ASP:HB3	2:B:27:LYS:HE2	1.86	0.57
2:D:224:ILE:HD11	2:D:336:SER:HB3	1.86	0.57
2:B:224:ILE:HD11	2:B:336:SER:HB3	1.86	0.57
1:A:359:ARG:O	1:A:363:VAL:HG22	2.04	0.57
2:D:231:GLU:HB3	2:D:237:PHE:CZ	2.39	0.57
2:D:370:TRP:HA	2:D:394:LEU:O	2.04	0.57
3:G:98:ALA:HB3	3:H:131:VAL:HB	1.85	0.57
1:C:85:PRO:HB2	7:D:525:CLF:S2B	2.44	0.57
3:E:244:ALA:O	3:E:248:VAL:HG23	2.04	0.57
1:C:332:LYS:O	1:C:336:GLU:HB2	2.04	0.56
1:A:52:SER:OG	1:A:60:ARG:HD2	2.06	0.56
1:A:85:PRO:HB2	7:B:525:CLF:S2B	2.45	0.56
2:B:95:CYS:HB3	2:B:99:PHE:CZ	2.40	0.56
1:C:106:VAL:HG21	2:D:40:ILE:HG23	1.86	0.56
1:A:60:ARG:HD3	1:A:190:SER:HB3	1.88	0.56
2:D:216:LYS:CG	2:D:285:PRO:HB2	2.36	0.56
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.88	0.56
1:C:60:ARG:HD3	1:C:190:SER:HB3	1.87	0.56
1:C:192:SER:OG	1:C:383:HIS:CE1	2.58	0.56
3:G:178:ARG:HB2	3:G:253:LEU:HB3	1.88	0.56
1:A:104:THR:HG21	1:A:111:THR:HB	1.88	0.56
3:F:178:ARG:HB2	3:F:253:LEU:HB3	1.87	0.56
1:A:192:SER:OG	1:A:383:HIS:CE1	2.58	0.56
1:C:52:SER:OG	1:C:60:ARG:HD2	2.06	0.56
1:C:394:MET:HG3	1:C:400:LEU:HD21	1.89	0.55
3:H:178:ARG:HB2	3:H:253:LEU:HB3	1.87	0.55
3:G:76:LEU:HD11	3:G:84:LYS:HB3	1.89	0.55
2:D:118:MET:HB2	2:D:154:MET:HE1	1.88	0.55
1:A:159:ILE:HG22	3:E:97:CYS:HB2	1.88	0.55
1:C:359:ARG:O	1:C:363:VAL:HG22	2.06	0.55
2:D:161:ASP:OD2	3:G:140:ARG:HG2	2.06	0.55
3:G:273:ILE:O	3:G:274:MET:HB2	2.07	0.55
1:A:155:PRO:HG3	2:B:153:CYS:HB2	1.89	0.55
1:C:155:PRO:HG3	2:D:153:CYS:HB2	1.87	0.55
2:B:478:HIS:O	2:B:481:ARG:HG3	2.06	0.54
2:D:478:HIS:O	2:D:481:ARG:HG3	2.07	0.54
2:D:277:THR:OG1	2:D:280:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.42	0.54
1:C:104:THR:HG21	1:C:111:THR:HB	1.88	0.54
3:H:76:LEU:HD11	3:H:84:LYS:HB3	1.90	0.54
3:F:273:ILE:O	3:F:274:MET:HB2	2.08	0.54
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.43	0.54
3:H:273:ILE:O	3:H:274:MET:HB2	2.08	0.54
1:C:256:ASP:HB3	2:D:27:LYS:HE2	1.90	0.54
2:B:369:LEU:HD22	2:B:379:LEU:HD13	1.90	0.53
1:C:346:LEU:HD21	1:C:464:ASP:HA	1.90	0.53
1:A:346:LEU:HD21	1:A:464:ASP:HA	1.89	0.53
2:B:277:THR:OG1	2:B:280:GLU:HG3	2.09	0.53
2:B:216:LYS:CG	2:B:285:PRO:HB2	2.36	0.53
1:A:198:ALA:O	1:A:202:VAL:HG23	2.09	0.53
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.57	0.53
2:D:164:ALA:HA	3:G:174:SER:HB2	1.91	0.53
2:B:118:MET:HB2	2:B:154:MET:HE1	1.89	0.53
1:C:198:ALA:O	1:C:202:VAL:HG23	2.08	0.53
2:D:72:PRO:HG3	7:D:525:CLF:S3B	2.49	0.53
3:F:76:LEU:HD11	3:F:84:LYS:HB3	1.89	0.53
1:A:46:ILE:HG23	1:A:46:ILE:O	2.09	0.53
2:B:379:LEU:HD11	2:B:443:ILE:HG21	1.91	0.53
2:D:202:GLU:HG3	2:D:300:LYS:HG2	1.91	0.53
1:A:346:LEU:CD2	1:A:467:LEU:HD23	2.39	0.53
1:C:346:LEU:CD2	1:C:467:LEU:HD23	2.38	0.53
1:C:70:VAL:HG11	5:C:496:CFM:S2B	2.48	0.53
1:A:55:GLY:HA2	2:B:114:VAL:HG11	1.90	0.52
1:A:394:MET:HG3	1:A:400:LEU:HD21	1.89	0.52
2:B:358:SER:OG	2:D:478:HIS:HE1	1.92	0.52
2:D:379:LEU:HD11	2:D:443:ILE:HG21	1.90	0.52
3:E:76:LEU:HD11	3:E:84:LYS:HB3	1.90	0.52
1:C:33:ALA:HB2	1:C:45:CYS:O	2.09	0.52
3:E:196:ILE:HB	3:E:207:MET:HE3	1.91	0.52
1:A:40:THR:O	1:A:41:GLN:HB2	2.09	0.52
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.45	0.52
3:H:196:ILE:HB	3:H:207:MET:HE3	1.92	0.52
1:A:239:ARG:HH11	1:A:252:GLN:HE21	1.55	0.52
1:A:226:ILE:HA	1:A:253:TRP:HB2	1.92	0.52
2:D:247:MET:HB2	2:D:249:VAL:HG23	1.92	0.52
1:A:70:VAL:HG11	5:A:496:CFM:S2B	2.50	0.52
2:B:445:ASN:HB2	2:B:472:PRO:O	2.10	0.52
1:A:33:ALA:HB2	1:A:45:CYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:GLU:HG3	2:B:300:LYS:HG2	1.91	0.52
2:B:247:MET:HB2	2:B:249:VAL:HG23	1.92	0.51
1:C:46:ILE:HG23	1:C:46:ILE:O	2.09	0.51
2:D:369:LEU:HD22	2:D:379:LEU:HD13	1.91	0.51
2:D:108:ARG:HG3	2:D:108:ARG:HH11	1.75	0.51
1:C:40:THR:O	1:C:41:GLN:HB2	2.10	0.51
3:E:273:ILE:O	3:E:274:MET:HB2	2.08	0.51
3:F:196:ILE:HB	3:F:207:MET:HE3	1.93	0.51
2:B:156:GLU:HG3	2:B:187:PRO:HA	1.93	0.51
3:H:11:GLY:HA2	3:H:128:GLY:HA3	1.93	0.51
1:A:51:LYS:HE3	3:F:65:GLY:HA2	1.93	0.51
2:D:156:GLU:HG3	2:D:187:PRO:HA	1.93	0.51
3:G:11:GLY:HA2	3:G:128:GLY:HA3	1.93	0.50
1:A:103:THR:HB	1:A:106:VAL:CG2	2.40	0.50
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.45	0.50
2:D:445:ASN:HB2	2:D:472:PRO:O	2.10	0.50
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.76	0.50
1:C:475:LEU:HD12	2:D:267:GLY:H	1.77	0.50
3:G:113:GLY:O	3:G:115:TYR:N	2.43	0.50
2:B:118:MET:CB	2:B:154:MET:HE1	2.42	0.50
2:D:118:MET:CB	2:D:154:MET:HE1	2.41	0.50
3:E:11:GLY:HA2	3:E:128:GLY:HA3	1.92	0.50
3:H:113:GLY:O	3:H:115:TYR:N	2.45	0.50
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.93	0.50
3:E:12:GLY:HA3	3:F:11:GLY:O	2.11	0.50
1:C:55:GLY:HA2	2:D:114:VAL:HG11	1.93	0.50
2:D:114:VAL:HG12	2:D:115:SER:N	2.26	0.50
2:B:114:VAL:HG12	2:B:115:SER:N	2.26	0.50
2:D:47:THR:HA	2:D:52:TYR:CG	2.47	0.50
2:D:473:ILE:HG21	2:D:479:LEU:HD12	1.93	0.50
3:E:11:GLY:O	3:F:12:GLY:HA3	2.12	0.50
1:C:85:PRO:HG3	2:D:189:PHE:HB3	1.94	0.50
1:C:157:GLY:CA	1:C:184:GLU:HG2	2.42	0.50
2:D:126:GLY:HA3	3:H:95:VAL:HG22	1.93	0.50
3:F:113:GLY:O	3:F:115:TYR:N	2.45	0.50
2:B:72:PRO:HG3	7:B:525:CLF:S3B	2.52	0.49
2:B:108:ARG:HG3	2:B:108:ARG:HH11	1.77	0.49
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.27	0.49
1:C:357:GLY:HA2	1:C:379:TYR:CD2	2.48	0.49
2:D:391:VAL:HA	2:D:419:ALA:HA	1.94	0.49
3:F:11:GLY:HA2	3:F:128:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:218:GLN:O	3:H:222:ILE:HG12	2.12	0.49
1:C:226:ILE:HA	1:C:253:TRP:HB2	1.93	0.49
1:A:387:TYR:O	1:A:391:MET:HG3	2.13	0.49
2:B:209:THR:HG21	2:B:309:TRP:CD1	2.47	0.49
2:B:494:LEU:O	2:B:498:VAL:HG23	2.12	0.49
3:G:218:GLN:O	3:G:222:ILE:HG12	2.12	0.49
3:H:162:ASN:HD21	3:H:259:ILE:H	1.60	0.49
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.27	0.49
2:B:305:VAL:O	2:B:309:TRP:HB2	2.12	0.49
2:D:397:ASN:ND2	2:D:397:ASN:H	2.10	0.49
3:E:113:GLY:O	3:E:115:TYR:N	2.45	0.49
1:A:332:LYS:HB3	1:A:333:PRO:HD3	1.94	0.49
3:G:50:HIS:O	3:G:224:ARG:HD3	2.13	0.49
2:B:391:VAL:HA	2:B:419:ALA:HA	1.95	0.49
2:B:473:ILE:HG21	2:B:479:LEU:HD12	1.94	0.49
2:D:494:LEU:O	2:D:498:VAL:HG23	2.12	0.49
2:B:397:ASN:H	2:B:397:ASN:ND2	2.10	0.49
1:C:332:LYS:HB3	1:C:333:PRO:HD3	1.93	0.49
1:C:387:TYR:O	1:C:391:MET:HG3	2.13	0.49
1:C:475:LEU:HD12	2:D:267:GLY:N	2.28	0.49
3:E:137:MET:HB3	3:E:138:PRO:HD3	1.95	0.49
3:E:218:GLN:O	3:E:222:ILE:HG12	2.12	0.49
3:F:162:ASN:HD21	3:F:259:ILE:H	1.61	0.49
3:F:218:GLN:O	3:F:222:ILE:HG12	2.12	0.49
1:A:7:GLU:CD	1:A:7:GLU:H	2.16	0.49
1:A:37:PRO:O	1:A:38:ALA:HB3	2.12	0.49
1:A:157:GLY:CA	1:A:184:GLU:HG2	2.42	0.49
1:A:381:PHE:CZ	5:A:496:CFM:S2B	3.05	0.49
2:B:47:THR:HA	2:B:52:TYR:CG	2.48	0.49
1:A:412:PHE:O	1:A:416:ILE:HG12	2.13	0.49
1:C:103:THR:HB	1:C:106:VAL:CG2	2.41	0.49
3:G:223:ARG:HD2	3:G:230:TYR:HE1	1.78	0.49
1:C:139:GLU:HG3	1:C:174:LEU:HD13	1.95	0.48
3:F:137:MET:HB3	3:F:138:PRO:HD3	1.95	0.48
2:B:88:TYR:OH	2:B:116:ASP:HB3	2.12	0.48
1:C:37:PRO:O	1:C:38:ALA:HB3	2.12	0.48
2:D:88:TYR:OH	2:D:116:ASP:HB3	2.13	0.48
3:E:33:VAL:HG22	3:E:121:PHE:HB2	1.95	0.48
3:E:162:ASN:HD21	3:E:259:ILE:H	1.61	0.48
1:C:412:PHE:O	1:C:416:ILE:HG12	2.13	0.48
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:CYS:O	2:B:157:VAL:HG23	2.14	0.48
1:C:48:SER:HB2	1:C:382:ALA:O	2.13	0.48
2:D:71:GLN:O	2:D:196:GLY:HA3	2.14	0.48
2:D:305:VAL:O	2:D:309:TRP:HB2	2.14	0.48
2:D:209:THR:HG21	2:D:309:TRP:CD1	2.48	0.48
3:E:130:VAL:HG23	3:E:135:PHE:HB2	1.96	0.48
2:D:104:ASN:ND2	2:D:111:VAL:HG23	2.28	0.48
1:A:106:VAL:O	1:A:144:LEU:HB2	2.14	0.48
2:B:104:ASN:ND2	2:B:111:VAL:HG23	2.29	0.48
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.96	0.48
3:G:196:ILE:HB	3:G:207:MET:HE3	1.96	0.48
1:C:381:PHE:CZ	5:C:496:CFM:S2B	3.07	0.48
3:H:38:CYS:HB2	3:H:126:VAL:HA	1.96	0.48
1:A:357:GLY:HA2	1:A:379:TYR:CD2	2.47	0.47
2:B:228:PRO:HA	2:B:293:LEU:HD12	1.96	0.47
2:B:512:MET:HE2	2:D:453:ARG:HG2	1.95	0.47
1:C:7:GLU:CD	1:C:7:GLU:H	2.16	0.47
1:C:77:ASP:HA	1:C:107:ASN:O	2.14	0.47
3:H:137:MET:HB3	3:H:138:PRO:HD3	1.95	0.47
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.96	0.47
2:D:88:TYR:O	2:D:149:VAL:HA	2.14	0.47
2:D:373:PRO:HD3	2:D:397:ASN:ND2	2.29	0.47
3:F:223:ARG:HD2	3:F:230:TYR:HE1	1.79	0.47
3:G:11:GLY:O	3:H:12:GLY:HA3	2.13	0.47
1:A:224:ALA:HB3	1:A:271:ASN:HD22	1.78	0.47
2:B:363:HIS:CG	1:C:465:MET:HG3	2.49	0.47
1:C:106:VAL:O	1:C:144:LEU:HB2	2.14	0.47
3:F:50:HIS:O	3:F:224:ARG:HD3	2.14	0.47
3:H:223:ARG:HD2	3:H:230:TYR:HE1	1.79	0.47
2:D:153:CYS:O	2:D:157:VAL:HG23	2.14	0.47
3:G:38:CYS:HB2	3:G:126:VAL:HA	1.96	0.47
3:G:130:VAL:HG23	3:G:135:PHE:HB2	1.95	0.47
3:G:162:ASN:HD21	3:G:259:ILE:H	1.61	0.47
1:A:77:ASP:HA	1:A:107:ASN:O	2.14	0.47
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.95	0.47
1:C:433:LYS:HE2	2:D:263:THR:OG1	2.14	0.47
3:E:223:ARG:HD2	3:E:230:TYR:HE1	1.79	0.47
3:F:33:VAL:HG22	3:F:121:PHE:HB2	1.96	0.47
3:F:130:VAL:HG23	3:F:135:PHE:HB2	1.96	0.47
3:G:33:VAL:HG22	3:G:121:PHE:HB2	1.96	0.47
3:G:137:MET:HB3	3:G:138:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:130:VAL:HG23	3:H:135:PHE:HB2	1.96	0.47
1:A:356:GLY:HA3	5:A:496:CFM:S1B	2.55	0.47
2:B:394:LEU:HD13	2:B:430:LEU:HB2	1.97	0.47
1:C:420:LEU:HD12	1:C:437:PRO:O	2.13	0.47
1:C:472:TRP:O	1:C:475:LEU:HD23	2.15	0.47
1:A:81:ILE:HD13	1:A:134:LEU:HD22	1.96	0.47
2:D:74:GLY:HA3	2:D:193:HIS:O	2.15	0.47
3:H:50:HIS:O	3:H:224:ARG:HD3	2.15	0.47
2:B:71:GLN:O	2:B:196:GLY:HA3	2.14	0.47
1:C:93:ARG:HD2	1:C:113:ASN:CB	2.45	0.47
1:A:48:SER:HB2	1:A:382:ALA:O	2.15	0.47
2:B:324:TRP:HH2	2:B:377:MET:HG2	1.80	0.46
2:D:180:PRO:HA	2:D:207:TYR:OH	2.15	0.46
2:D:258:GLU:HG3	2:D:259:GLU:N	2.30	0.46
3:E:50:HIS:O	3:E:224:ARG:HD3	2.14	0.46
3:F:38:CYS:HB2	3:F:126:VAL:HA	1.96	0.46
3:H:256:PRO:O	3:H:258:PRO:HD3	2.15	0.46
1:A:472:TRP:O	1:A:475:LEU:HD23	2.15	0.46
2:B:158:ILE:HG22	3:F:97:CYS:CB	2.33	0.46
2:B:74:GLY:HA3	2:B:193:HIS:O	2.16	0.46
2:B:158:ILE:CG2	3:F:97:CYS:HB2	2.32	0.46
3:E:38:CYS:HB2	3:E:126:VAL:HA	1.96	0.46
3:H:45:THR:CG2	3:H:85:CYS:HB3	2.44	0.46
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.96	0.46
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.51	0.46
2:B:180:PRO:HA	2:B:207:TYR:OH	2.15	0.46
2:B:451:ILE:O	2:B:455:THR:HG23	2.15	0.46
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.97	0.46
2:B:88:TYR:O	2:B:149:VAL:HA	2.15	0.46
2:B:373:PRO:HD3	2:B:397:ASN:ND2	2.31	0.46
1:A:210:ARG:HG3	1:A:263:GLU:HB3	1.98	0.46
1:A:420:LEU:HD12	1:A:437:PRO:O	2.16	0.46
2:B:258:GLU:HG3	2:B:259:GLU:N	2.29	0.46
1:C:81:ILE:HD13	1:C:134:LEU:HD22	1.96	0.46
1:C:356:GLY:HA3	5:C:496:CFM:S1B	2.56	0.46
3:H:1:ALA:O	3:H:2:MET:HB3	2.15	0.46
3:E:22:LEU:HD13	3:E:243:LEU:HG	1.97	0.46
3:F:56:THR:O	3:F:60:MET:HB2	2.16	0.46
1:A:93:ARG:HD2	1:A:113:ASN:CB	2.45	0.46
2:B:131:MET:HG2	2:B:165:PHE:HB3	1.96	0.46
2:B:472:PRO:HB2	2:B:474:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:GLN:CG	1:C:42:SER:H	2.28	0.46
3:E:256:PRO:O	3:E:258:PRO:HD3	2.16	0.46
3:H:131:VAL:HG23	3:H:132:CYS:SG	2.56	0.46
3:G:1:ALA:O	3:G:2:MET:HB3	2.16	0.46
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.98	0.45
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.51	0.45
2:D:131:MET:HG2	2:D:165:PHE:HB3	1.97	0.45
2:D:472:PRO:HB2	2:D:474:PHE:CE1	2.52	0.45
3:F:45:THR:CG2	3:F:85:CYS:HB3	2.45	0.45
1:C:11:SER:O	1:C:15:GLU:HG3	2.16	0.45
1:C:187:ARG:HA	2:D:120:GLU:HG2	1.98	0.45
2:D:198:ASP:HB2	2:D:297:HIS:O	2.16	0.45
3:G:86:VAL:HG11	3:G:109:LEU:HD21	1.98	0.45
3:G:126:VAL:HG12	3:G:127:LEU:HD23	1.98	0.45
1:A:263:GLU:O	1:A:266:PRO:HD2	2.17	0.45
3:H:22:LEU:HD13	3:H:243:LEU:HG	1.99	0.45
3:H:86:VAL:HG11	3:H:109:LEU:HD21	1.98	0.45
1:A:148:ILE:HG22	1:A:149:SER:N	2.31	0.45
1:A:275:CYS:SG	1:A:278:SER:OG	2.67	0.45
3:G:22:LEU:HD13	3:G:243:LEU:HG	1.98	0.45
1:C:229:TYR:CD1	1:C:254:SER:HB2	2.51	0.45
2:D:305:VAL:HG12	2:D:311:HIS:HB2	1.99	0.45
3:F:256:PRO:O	3:F:258:PRO:HD3	2.17	0.45
1:C:62:CYS:HB2	1:C:185:GLY:CA	2.46	0.45
3:F:86:VAL:HG11	3:F:109:LEU:HD21	1.98	0.45
1:A:41:GLN:CG	1:A:42:SER:H	2.29	0.45
2:B:118:MET:SD	2:B:154:MET:HE1	2.57	0.45
1:C:394:MET:HB3	1:C:398:THR:OG1	2.16	0.45
2:D:118:MET:SD	2:D:154:MET:HE1	2.57	0.45
2:D:324:TRP:HH2	2:D:377:MET:HG2	1.81	0.45
2:D:451:ILE:O	2:D:455:THR:HG23	2.17	0.45
3:E:1:ALA:O	3:E:2:MET:HB3	2.16	0.45
3:E:86:VAL:HG11	3:E:109:LEU:HD21	1.98	0.45
3:G:159:TYR:HE1	3:H:41:LYS:HB3	1.80	0.45
1:A:93:ARG:HD2	1:A:113:ASN:HB2	1.98	0.45
2:B:71:GLN:N	2:B:72:PRO:HD2	2.31	0.45
1:C:93:ARG:HD2	1:C:113:ASN:HB2	1.99	0.45
3:E:56:THR:O	3:E:60:MET:HB2	2.16	0.45
2:B:198:ASP:HB2	2:B:297:HIS:O	2.16	0.45
1:C:148:ILE:HG22	1:C:149:SER:N	2.31	0.45
2:D:124:VAL:O	3:H:96:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:ALA:O	3:F:2:MET:HB3	2.16	0.45
3:H:126:VAL:HG12	3:H:127:LEU:HD23	1.99	0.45
2:B:328:PHE:O	2:B:332:VAL:HG23	2.17	0.45
2:D:71:GLN:N	2:D:72:PRO:HD2	2.32	0.45
3:H:33:VAL:HG22	3:H:121:PHE:HB2	1.97	0.45
1:A:302:PRO:HG2	1:A:369:ASP:OD2	2.17	0.44
1:A:422:GLY:HA2	1:A:439:ARG:O	2.17	0.44
1:C:263:GLU:O	1:C:266:PRO:HD2	2.17	0.44
3:G:256:PRO:O	3:G:258:PRO:HD3	2.17	0.44
1:A:177:THR:OG1	1:A:209:LYS:HE3	2.18	0.44
1:A:420:LEU:HD21	1:A:463:MET:HE2	1.98	0.44
1:C:66:GLY:O	1:C:70:VAL:HG22	2.18	0.44
1:C:422:GLY:HA2	1:C:439:ARG:O	2.18	0.44
3:F:260:THR:OG1	3:F:263:GLU:HG3	2.17	0.44
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.44	0.44
1:A:62:CYS:HB2	1:A:185:GLY:CA	2.46	0.44
1:A:85:PRO:HG3	2:B:189:PHE:HB3	1.99	0.44
1:A:394:MET:HB3	1:A:398:THR:OG1	2.17	0.44
2:B:161:ASP:OD2	3:E:140:ARG:HG2	2.17	0.44
3:F:22:LEU:HD13	3:F:243:LEU:HG	1.98	0.44
3:F:126:VAL:HG12	3:F:127:LEU:HD23	1.99	0.44
3:G:56:THR:O	3:G:60:MET:HB2	2.16	0.44
1:C:302:PRO:HG2	1:C:369:ASP:OD2	2.18	0.44
2:D:156:GLU:HG3	2:D:187:PRO:CA	2.48	0.44
1:A:86:VAL:O	7:B:525:CLF:S2B	2.75	0.44
3:G:260:THR:OG1	3:G:263:GLU:HG3	2.17	0.44
1:A:229:TYR:CD1	1:A:254:SER:HB2	2.52	0.44
1:A:275:CYS:CA	1:A:358:LEU:HD22	2.42	0.44
1:A:351:VAL:O	1:A:374:VAL:HA	2.18	0.44
2:B:86:MET:SD	2:B:114:VAL:HG23	2.58	0.44
2:B:293:LEU:O	2:B:318:ILE:HA	2.18	0.44
2:D:328:PHE:O	2:D:332:VAL:HG23	2.17	0.44
2:B:453:ARG:HG2	2:D:512:MET:HE2	1.99	0.44
2:B:156:GLU:HG3	2:B:187:PRO:CA	2.48	0.44
1:C:442:HIS:CG	4:C:494:HCA:H51	2.53	0.44
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.45	0.44
3:H:19:THR:O	3:H:23:VAL:HG23	2.18	0.44
2:B:381:LYS:O	2:B:385:GLU:HG3	2.18	0.43
2:B:487:TYR:O	2:B:491:MET:HG3	2.17	0.43
1:C:86:VAL:O	2:D:70:CYS:HB3	2.17	0.43
3:E:260:THR:OG1	3:E:263:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:MET:HE3	2:D:457:HIS:HB2	2.01	0.43
3:E:126:VAL:HG12	3:E:127:LEU:HD23	1.99	0.43
3:F:56:THR:OG1	3:F:59:GLU:HB2	2.18	0.43
1:A:11:SER:O	1:A:15:GLU:HG3	2.17	0.43
1:A:106:VAL:CG2	2:B:40:ILE:HG23	2.47	0.43
2:B:200:MET:O	2:B:204:ILE:HG13	2.18	0.43
2:B:457:HIS:HB2	2:D:512:MET:HE3	2.00	0.43
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.59	0.43
2:D:373:PRO:HG3	2:D:395:CYS:SG	2.59	0.43
3:E:139:ILE:HG13	3:E:147:ILE:HD11	2.01	0.43
3:G:196:ILE:HB	3:G:207:MET:CE	2.48	0.43
2:B:324:TRP:CZ3	2:B:378:GLY:HA2	2.53	0.43
1:C:210:ARG:HG3	1:C:263:GLU:HB3	2.00	0.43
2:D:324:TRP:CZ3	2:D:378:GLY:HA2	2.54	0.43
3:F:196:ILE:HB	3:F:207:MET:CE	2.48	0.43
3:G:19:THR:O	3:G:23:VAL:HG23	2.19	0.43
1:A:144:LEU:CD1	2:B:43:VAL:HG21	2.48	0.43
1:A:231:ILE:HG22	1:A:444:TRP:CD1	2.53	0.43
1:C:203:ARG:HG3	1:C:285:HIS:CE1	2.54	0.43
1:A:203:ARG:HG3	1:A:285:HIS:CE1	2.53	0.43
1:C:275:CYS:CA	1:C:358:LEU:HD22	2.41	0.43
1:C:300:PHE:CD1	1:C:363:VAL:HG12	2.54	0.43
1:C:343:ARG:HB3	1:C:344:PRO:HD3	2.01	0.43
1:C:425:ILE:HD12	2:D:104:ASN:HB3	2.00	0.43
2:D:381:LYS:O	2:D:385:GLU:HG3	2.19	0.43
2:D:463:GLU:HB3	2:D:504:ARG:HH21	1.83	0.43
3:H:196:ILE:HB	3:H:207:MET:CE	2.48	0.43
1:A:280:ASN:ND2	1:A:284:ARG:NH1	2.67	0.43
3:F:139:ILE:HG13	3:F:147:ILE:HD11	2.01	0.43
3:F:146:GLU:HA	3:F:178:ARG:O	2.19	0.43
3:G:131:VAL:HG23	3:G:132:CYS:SG	2.59	0.43
3:H:56:THR:OG1	3:H:59:GLU:HB2	2.18	0.43
3:H:56:THR:O	3:H:60:MET:HB2	2.18	0.43
3:H:67:VAL:HG21	3:H:104:THR:HG21	2.00	0.43
2:B:463:GLU:HB3	2:B:504:ARG:HH21	1.84	0.43
1:C:334:GLU:O	1:C:338:VAL:HG23	2.18	0.43
3:F:178:ARG:HA	3:F:178:ARG:HD3	1.85	0.43
1:A:245:MET:HB3	1:A:327:VAL:HG21	2.00	0.43
1:C:184:GLU:HB3	1:C:186:PHE:CE2	2.54	0.43
1:C:265:THR:HG22	1:C:286:MET:CE	2.49	0.43
2:D:200:MET:O	2:D:204:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLY:O	1:A:70:VAL:HG22	2.18	0.43
1:A:265:THR:HG22	1:A:286:MET:CE	2.49	0.43
1:A:334:GLU:O	1:A:338:VAL:HG23	2.18	0.43
2:B:305:VAL:HG12	2:B:311:HIS:HB2	2.00	0.43
1:C:351:VAL:O	1:C:374:VAL:HA	2.19	0.43
3:E:67:VAL:HG21	3:E:104:THR:HG21	2.00	0.43
3:G:49:LEU:CD1	3:G:53:ALA:HB2	2.49	0.43
3:H:139:ILE:HG13	3:H:147:ILE:HD11	2.00	0.43
1:A:79:ILE:O	1:A:148:ILE:HA	2.19	0.42
2:B:12:TYR:OH	2:D:508:GLU:HB3	2.19	0.42
1:C:54:PRO:HB3	2:D:116:ASP:O	2.19	0.42
3:E:93:PRO:HB3	3:F:130:VAL:HG13	2.00	0.42
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.59	0.42
1:C:177:THR:OG1	1:C:209:LYS:HE3	2.19	0.42
2:D:41:ASP:O	2:D:45:GLN:HG2	2.19	0.42
3:F:49:LEU:CD1	3:F:53:ALA:HB2	2.49	0.42
3:G:25:ALA:O	3:G:29:MET:HG3	2.18	0.42
3:H:146:GLU:HA	3:H:178:ARG:O	2.19	0.42
1:A:438:PHE:CD1	1:A:439:ARG:N	2.87	0.42
1:C:79:ILE:O	1:C:148:ILE:HA	2.19	0.42
2:D:293:LEU:O	2:D:318:ILE:HA	2.19	0.42
3:E:146:GLU:HA	3:E:178:ARG:O	2.19	0.42
3:F:131:VAL:HG23	3:F:132:CYS:SG	2.60	0.42
3:G:56:THR:OG1	3:G:59:GLU:HB2	2.19	0.42
1:C:20:TYR:HA	1:C:21:PRO:HD3	1.95	0.42
1:C:86:VAL:O	7:D:525:CLF:S2B	2.78	0.42
1:C:350:ARG:HD2	1:C:375:VAL:HG21	2.02	0.42
3:E:19:THR:O	3:E:23:VAL:HG23	2.19	0.42
3:H:260:THR:OG1	3:H:263:GLU:HG3	2.18	0.42
1:C:44:LYS:HE2	1:C:44:LYS:HA	2.01	0.42
2:D:441:PHE:CZ	2:D:501:ILE:HA	2.54	0.42
2:D:487:TYR:O	2:D:491:MET:HG3	2.18	0.42
1:A:30:LYS:HB3	1:A:47:ILE:HG22	2.01	0.42
1:A:70:VAL:HG23	1:A:71:VAL:HG23	2.01	0.42
1:A:475:LEU:HD12	2:B:267:GLY:H	1.85	0.42
2:B:41:ASP:O	2:B:45:GLN:HG2	2.20	0.42
2:B:478:HIS:HE1	2:D:358:SER:OG	2.02	0.42
1:C:229:TYR:CE1	1:C:254:SER:HB2	2.54	0.42
1:C:438:PHE:CD1	1:C:439:ARG:N	2.87	0.42
2:D:197:TRP:CZ3	2:D:229:GLY:HA2	2.55	0.42
2:D:441:PHE:HD2	2:D:465:PRO:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:56:THR:OG1	3:E:59:GLU:HB2	2.19	0.42
3:F:67:VAL:HG21	3:F:104:THR:HG21	2.00	0.42
3:G:146:GLU:HA	3:G:178:ARG:O	2.20	0.42
3:H:49:LEU:CD1	3:H:53:ALA:HB2	2.49	0.42
1:A:223:VAL:HG11	1:A:247:LEU:HD13	2.00	0.42
1:A:417:LYS:N	1:A:418:PRO:HD3	2.35	0.42
2:B:441:PHE:HD2	2:B:465:PRO:HB2	1.84	0.42
2:B:446:SER:OG	2:B:473:ILE:HA	2.19	0.42
1:C:70:VAL:HG23	1:C:71:VAL:HG23	2.02	0.42
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.55	0.42
1:A:44:LYS:HE2	1:A:44:LYS:HA	2.01	0.42
1:A:184:GLU:HB3	1:A:186:PHE:CE2	2.54	0.42
1:A:442:HIS:CG	4:A:494:HCA:H51	2.54	0.42
2:B:70:CYS:SG	2:B:72:PRO:HG2	2.60	0.42
2:D:441:PHE:CD2	2:D:465:PRO:HB2	2.55	0.42
2:B:441:PHE:CZ	2:B:501:ILE:HA	2.55	0.42
1:C:280:ASN:ND2	1:C:284:ARG:NH1	2.68	0.42
1:C:352:MET:SD	1:C:418:PRO:CG	3.08	0.42
3:F:25:ALA:O	3:F:29:MET:HG3	2.19	0.42
3:H:49:LEU:HD12	3:H:53:ALA:HB2	2.01	0.42
3:H:144:ALA:O	3:H:177:VAL:HG22	2.20	0.42
1:C:30:LYS:HB3	1:C:47:ILE:HG22	2.02	0.42
1:C:40:THR:HG22	1:C:392:LYS:HE3	2.02	0.42
1:C:229:TYR:HA	1:C:254:SER:O	2.19	0.42
1:C:245:MET:HB3	1:C:327:VAL:HG21	2.01	0.42
3:F:19:THR:O	3:F:23:VAL:HG23	2.20	0.42
3:G:13:ILE:HD12	3:G:13:ILE:HA	1.93	0.42
1:A:229:TYR:CE1	1:A:254:SER:HB2	2.55	0.41
1:C:144:LEU:HD13	2:D:43:VAL:HG21	2.02	0.41
1:C:231:ILE:HG22	1:C:444:TRP:CD1	2.54	0.41
1:C:477:ALA:HA	1:C:478:PRO:HD3	1.91	0.41
3:E:49:LEU:CD1	3:E:53:ALA:HB2	2.50	0.41
3:E:196:ILE:HB	3:E:207:MET:CE	2.49	0.41
1:A:229:TYR:HA	1:A:254:SER:O	2.20	0.41
1:C:106:VAL:CG2	2:D:40:ILE:HG23	2.50	0.41
1:C:275:CYS:SG	1:C:278:SER:OG	2.68	0.41
3:G:49:LEU:HD12	3:G:53:ALA:HB2	2.02	0.41
3:G:159:TYR:CE1	3:H:41:LYS:HB3	2.54	0.41
2:D:212:SER:O	2:D:216:LYS:HD3	2.20	0.41
3:E:49:LEU:HD12	3:E:53:ALA:HB2	2.02	0.41
3:E:131:VAL:HG23	3:E:132:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:221:GLU:CD	3:H:155:MET:HB3	2.41	0.41
3:H:25:ALA:O	3:H:29:MET:HG3	2.20	0.41
2:B:43:VAL:O	2:B:47:THR:HG23	2.20	0.41
1:C:442:HIS:HA	5:C:496:CFM:S4B	2.59	0.41
2:D:96:VAL:O	2:D:100:ARG:HG3	2.21	0.41
2:D:397:ASN:N	2:D:397:ASN:HD22	2.18	0.41
2:D:446:SER:OG	2:D:473:ILE:HA	2.21	0.41
1:A:86:VAL:O	2:B:70:CYS:HB3	2.21	0.41
2:D:86:MET:SD	2:D:114:VAL:HG23	2.60	0.41
3:E:130:VAL:HG13	3:F:93:PRO:HB3	2.02	0.41
2:B:397:ASN:HD22	2:B:397:ASN:N	2.18	0.41
3:H:209:HIS:HB3	3:H:243:LEU:HD13	2.03	0.41
1:A:352:MET:SD	1:A:418:PRO:CG	3.09	0.41
2:D:422:TYR:HB3	2:D:425:LYS:HG3	2.02	0.41
3:G:178:ARG:CB	3:G:253:LEU:HB3	2.51	0.41
1:A:274:HIS:HD2	1:A:297:TYR:CE2	2.39	0.41
2:B:422:TYR:HB3	2:B:425:LYS:HG3	2.01	0.41
2:D:71:GLN:HA	2:D:193:HIS:HA	2.03	0.41
2:D:301:THR:O	2:D:305:VAL:HG23	2.21	0.41
3:H:66:THR:HG22	3:H:68:GLU:H	1.85	0.41
2:B:197:TRP:CZ3	2:B:229:GLY:HA2	2.56	0.41
2:B:397:ASN:ND2	2:B:397:ASN:N	2.68	0.41
1:C:9:VAL:O	1:C:12:LEU:HB3	2.21	0.41
1:C:223:VAL:HG11	1:C:247:LEU:HD13	2.01	0.41
1:C:417:LYS:N	1:C:418:PRO:HD3	2.35	0.41
2:D:413:SER:HA	2:D:414:PRO:HD3	1.92	0.41
3:G:139:ILE:HG13	3:G:147:ILE:HD11	2.02	0.41
3:G:178:ARG:HA	3:G:178:ARG:HD3	1.84	0.41
1:A:9:VAL:O	1:A:12:LEU:HB3	2.21	0.41
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.21	0.41
2:B:72:PRO:O	2:B:76:VAL:HG23	2.21	0.41
2:D:72:PRO:O	2:D:76:VAL:HG23	2.21	0.41
3:G:66:THR:HG22	3:G:68:GLU:H	1.86	0.41
3:G:67:VAL:HG21	3:G:104:THR:HG21	2.02	0.41
3:G:139:ILE:O	3:G:139:ILE:HG12	2.21	0.41
1:A:475:LEU:HD12	2:B:267:GLY:N	2.36	0.40
3:E:206:GLN:NE2	3:E:252:LEU:HB3	2.36	0.40
3:F:66:THR:HG22	3:F:68:GLU:H	1.86	0.40
3:F:178:ARG:CB	3:F:253:LEU:HB3	2.51	0.40
3:F:209:HIS:HB3	3:F:243:LEU:HD13	2.04	0.40
2:B:380:VAL:HG13	2:B:390:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:PHE:CD2	2:B:465:PRO:HB2	2.56	0.40
2:D:397:ASN:ND2	2:D:397:ASN:N	2.68	0.40
3:E:25:ALA:O	3:E:29:MET:HG3	2.20	0.40
3:E:178:ARG:CB	3:E:253:LEU:HB3	2.51	0.40
3:F:139:ILE:HG12	3:F:139:ILE:O	2.20	0.40
3:H:178:ARG:CB	3:H:253:LEU:HB3	2.51	0.40
1:A:54:PRO:HB3	2:B:116:ASP:O	2.22	0.40
1:A:123:ILE:HD12	1:A:123:ILE:N	2.36	0.40
1:C:76:LYS:HD3	1:C:256:ASP:OD1	2.22	0.40
2:D:380:VAL:HG13	2:D:390:PRO:HG3	2.03	0.40
2:D:43:VAL:O	2:D:47:THR:HG23	2.21	0.40
3:E:76:LEU:CD1	3:E:86:VAL:HG22	2.48	0.40
3:E:144:ALA:O	3:E:177:VAL:HG22	2.21	0.40
3:F:49:LEU:HD12	3:F:53:ALA:HB2	2.02	0.40
3:G:209:HIS:HB3	3:G:243:LEU:HD13	2.03	0.40
1:A:343:ARG:HB3	1:A:344:PRO:HD3	2.03	0.40
3:E:242:ALA:O	3:E:246:LYS:HG2	2.22	0.40
3:H:228:ILE:HD13	3:H:237:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/491 (97%)	424 (89%)	42 (9%)	10 (2%)	7	33
1	C	476/491 (97%)	425 (89%)	42 (9%)	9 (2%)	8	36
2	B	520/522 (100%)	481 (92%)	35 (7%)	4 (1%)	19	57
2	D	520/522 (100%)	481 (92%)	35 (7%)	4 (1%)	19	57
3	E	272/289 (94%)	249 (92%)	19 (7%)	4 (2%)	10	42
3	F	272/289 (94%)	249 (92%)	19 (7%)	4 (2%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	272/289 (94%)	249 (92%)	19 (7%)	4 (2%)	10	42
3	H	272/289 (94%)	249 (92%)	19 (7%)	4 (2%)	10	42
All	All	3080/3182 (97%)	2807 (91%)	230 (8%)	43 (1%)	11	43

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	C	45	CYS
3	E	114	ALA
3	E	190	ASP
3	F	114	ALA
3	F	190	ASP
3	G	114	ALA
3	G	190	ASP
3	H	114	ALA
3	H	190	ASP
1	A	41	GLN
1	C	41	GLN
3	E	116	GLU
3	F	116	GLU
3	G	116	GLU
3	H	116	GLU
1	A	5	SER
1	A	428	LYS
2	B	210	LEU
2	B	322	LEU
1	C	5	SER
1	C	428	LYS
2	D	210	LEU
3	E	141	GLU
3	F	141	GLU
3	G	141	GLU
3	H	141	GLU
1	A	358	LEU
1	C	76	LYS
1	C	358	LEU
2	D	322	LEU
1	A	76	LYS
2	B	255	SER
2	D	255	SER

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Mol	Chain	Res	Type
1	A	22	GLU
1	A	355	ILE
1	C	355	ILE
2	B	5	VAL
2	D	5	VAL
1	A	126	GLY
1	A	356	GLY
1	C	126	GLY
1	C	356	GLY

5.3.2 Protein sidechains (i)

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	406/414 (98%)	392 (97%)	14 (3%)	37	72
1	C	406/414 (98%)	391 (96%)	15 (4%)	34	70
2	B	453/454 (100%)	441 (97%)	12 (3%)	46	78
2	D	453/454 (100%)	441 (97%)	12 (3%)	46	78
3	E	218/233 (94%)	208 (95%)	10 (5%)	27	64
3	F	218/233 (94%)	208 (95%)	10 (5%)	27	64
3	G	218/233 (94%)	208 (95%)	10 (5%)	27	64
3	H	218/233 (94%)	208 (95%)	10 (5%)	27	64
All	All	2590/2668 (97%)	2497 (96%)	93 (4%)	35	70

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	41	GLN
1	A	58	THR
1	A	128	ASP
1	A	131	LEU
1	A	176	LYS

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Mol	Chain	Res	Type
1	A	196	HIS
1	A	280	ASN
1	A	361	ARG
1	A	362	HIS
1	A	383	HIS
1	A	409	PHE
1	A	425	ILE
1	A	463	MET
2	B	31	PHE
2	B	37	GLN
2	B	88	TYR
2	B	151	THR
2	B	153	CYS
2	B	360	THR
2	B	379	LEU
2	B	383	LEU
2	B	397	ASN
2	B	420	THR
2	B	505	LEU
2	B	519	HIS
1	C	14	GLN
1	C	41	GLN
1	C	58	THR
1	C	128	ASP
1	C	131	LEU
1	C	176	LYS
1	C	196	HIS
1	C	280	ASN
1	C	361	ARG
1	C	362	HIS
1	C	369	ASP
1	C	383	HIS
1	C	409	PHE
1	C	425	ILE
1	C	463	MET
2	D	31	PHE
2	D	37	GLN
2	D	88	TYR
2	D	151	THR
2	D	153	CYS
2	D	360	THR
2	D	379	LEU

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Mol	Chain	Res	Type
2	D	383	LEU
2	D	397	ASN
2	D	420	THR
2	D	505	LEU
2	D	519	HIS
3	E	2	MET
3	E	59	GLU
3	E	73	GLU
3	E	86	VAL
3	E	117	ASP
3	E	132	CYS
3	E	155	MET
3	E	207	MET
3	E	257	ASN
3	E	274	MET
3	F	2	MET
3	F	59	GLU
3	F	73	GLU
3	F	86	VAL
3	F	117	ASP
3	F	132	CYS
3	F	155	MET
3	F	207	MET
3	F	257	ASN
3	F	274	MET
3	G	2	MET
3	G	59	GLU
3	G	73	GLU
3	G	86	VAL
3	G	117	ASP
3	G	132	CYS
3	G	155	MET
3	G	207	MET
3	G	257	ASN
3	G	274	MET
3	H	2	MET
3	H	59	GLU
3	H	73	GLU
3	H	86	VAL
3	H	117	ASP
3	H	132	CYS
3	H	155	MET

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Mol	Chain	Res	Type
3	H	207	MET
3	H	257	ASN
3	H	274	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	49	ASN
1	A	252	GLN
1	A	271	ASN
1	A	274	HIS
1	A	280	ASN
1	A	362	HIS
1	A	383	HIS
2	B	167	ASN
2	B	199	ASN
2	B	397	ASN
2	B	478	HIS
2	B	499	ASN
2	B	518	ASN
1	C	14	GLN
1	C	29	ASN
1	C	49	ASN
1	C	252	GLN
1	C	271	ASN
1	C	274	HIS
1	C	280	ASN
1	C	362	HIS
1	C	383	HIS
2	D	167	ASN
2	D	199	ASN
2	D	397	ASN
2	D	478	HIS
2	D	499	ASN
2	D	518	ASN
3	E	4	GLN
3	E	54	GLN
3	E	142	ASN
3	E	162	ASN
3	E	201	ASN

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Mol	Chain	Res	Type
3	E	206	GLN
3	F	4	GLN
3	F	54	GLN
3	F	162	ASN
3	F	201	ASN
3	F	206	GLN
3	G	4	GLN
3	G	54	GLN
3	G	142	ASN
3	G	162	ASN
3	G	201	ASN
3	G	206	GLN
3	H	4	GLN
3	H	54	GLN
3	H	142	ASN
3	H	162	ASN
3	H	201	ASN
3	H	206	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
9	ALF	G	293	-	0,4,4	0.00	-	-		
5	CFM	C	496	1	0,24,24	0.00	-	-		
11	SF4	G	290	3	0,12,12	0.00	-	-		
9	ALF	E	293	-	0,4,4	0.00	-	-		
4	HCA	A	494	-	4,13,13	0.84	0	4,18,18	0.93	0
9	ALF	F	293	-	0,4,4	0.00	-	-		
10	ADP	E	291	-	24,29,29	1.19	3 (12%)	29,45,45	2.20	6 (20%)
9	ALF	H	293	-	0,4,4	0.00	-	-		
10	ADP	H	291	-	24,29,29	1.29	3 (12%)	29,45,45	2.22	8 (27%)
7	CLF	D	525	1,2	0,24,24	0.00	-	-		
5	CFM	A	496	1	0,24,24	0.00	-	-		
7	CLF	B	525	1,2	0,24,24	0.00	-	-		
11	SF4	F	290	3	0,12,12	0.00	-	-		
4	HCA	C	494	-	4,13,13	0.88	0	4,18,18	0.92	0
10	ADP	G	291	-	24,29,29	1.24	3 (12%)	29,45,45	2.17	8 (27%)
10	ADP	F	291	-	24,29,29	1.18	2 (8%)	29,45,45	2.20	7 (24%)

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
11	SF4	G	290	3	-	-	0/6/5/5
4	HCA	A	494	-	-	1/7/17/17	-
10	ADP	E	291	-	-	0/12/32/32	0/3/3/3
10	ADP	H	291	-	-	0/12/32/32	0/3/3/3
7	CLF	D	525	1,2	-	-	0/12/10/10
11	SF4	F	290	3	-	-	0/6/5/5
7	CLF	B	525	1,2	-	-	0/12/10/10
4	HCA	C	494	-	-	1/7/17/17	-
10	ADP	G	291	-	-	0/12/32/32	0/3/3/3
10	ADP	F	291	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	291	ADP	O4'-C1'	3.54	1.46	1.41
10	G	291	ADP	O4'-C1'	2.88	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	291	ADP	O4'-C1'	2.70	1.44	1.41
10	G	291	ADP	PB-O2B	-2.65	1.44	1.54
10	F	291	ADP	PB-O2B	-2.60	1.44	1.54
10	F	291	ADP	O4'-C1'	2.40	1.44	1.41
10	H	291	ADP	PB-O2B	-2.34	1.45	1.54
10	E	291	ADP	PB-O2B	-2.34	1.45	1.54
10	G	291	ADP	C8-N7	-2.32	1.30	1.34
10	H	291	ADP	C8-N7	-2.25	1.30	1.34
10	E	291	ADP	C8-N7	-2.18	1.30	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	291	ADP	O4'-C1'-C2'	-7.42	96.08	106.93
10	H	291	ADP	O4'-C1'-C2'	-7.23	96.36	106.93
10	F	291	ADP	O4'-C1'-C2'	-7.16	96.47	106.93
10	G	291	ADP	O4'-C1'-C2'	-7.04	96.64	106.93
10	F	291	ADP	C2'-C3'-C4'	-5.00	92.93	102.64
10	H	291	ADP	C2'-C3'-C4'	-4.97	92.99	102.64
10	E	291	ADP	C2'-C3'-C4'	-4.93	93.06	102.64
10	G	291	ADP	C2'-C3'-C4'	-4.77	93.38	102.64
10	H	291	ADP	O3B-PB-O2B	-3.69	93.52	107.64
10	F	291	ADP	O3B-PB-O2B	-3.62	93.79	107.64
10	G	291	ADP	O3B-PB-O2B	-3.58	93.96	107.64
10	E	291	ADP	O3B-PB-O2B	-3.58	93.97	107.64
10	H	291	ADP	PA-O3A-PB	-3.35	121.34	132.83
10	E	291	ADP	PA-O3A-PB	-3.29	121.53	132.83
10	G	291	ADP	PA-O3A-PB	-3.26	121.62	132.83
10	F	291	ADP	PA-O3A-PB	-3.20	121.84	132.83
10	H	291	ADP	O3'-C3'-C2'	-3.04	101.97	111.82
10	G	291	ADP	O3'-C3'-C2'	-3.03	102.00	111.82
10	F	291	ADP	O3'-C3'-C2'	-2.98	102.19	111.82
10	E	291	ADP	O3'-C3'-C2'	-2.90	102.42	111.82
10	F	291	ADP	O5'-C5'-C4'	2.67	118.18	108.99
10	E	291	ADP	O5'-C5'-C4'	2.62	118.02	108.99
10	G	291	ADP	O5'-C5'-C4'	2.56	117.82	108.99
10	H	291	ADP	O5'-C5'-C4'	2.49	117.55	108.99
10	H	291	ADP	O3'-C3'-C4'	2.25	117.55	111.05
10	G	291	ADP	C5-C6-N6	2.21	123.72	120.35
10	G	291	ADP	O3'-C3'-C4'	2.18	117.35	111.05
10	H	291	ADP	C5-C6-N6	2.14	123.60	120.35
10	F	291	ADP	O3'-C3'-C4'	2.11	117.15	111.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	494	HCA	C3-C4-C5-C6
4	C	494	HCA	C3-C4-C5-C6

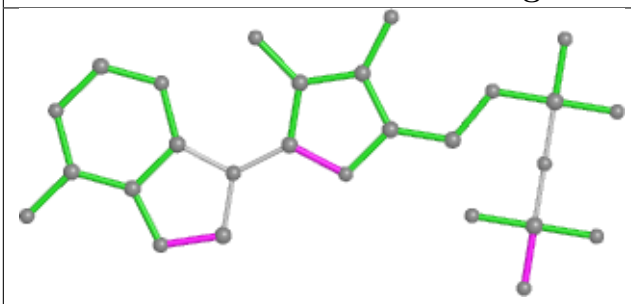
There are no ring outliers.

10 monomers are involved in 31 short contacts:

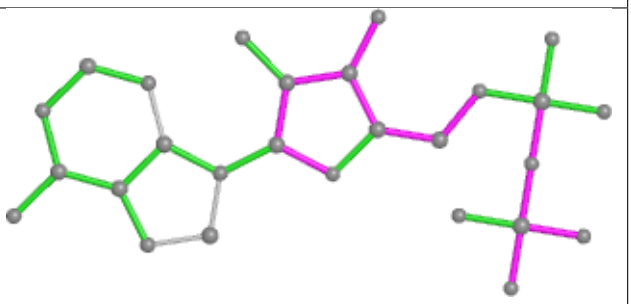
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	496	CFM	7	0
4	A	494	HCA	1	0
10	E	291	ADP	2	0
10	H	291	ADP	2	0
7	D	525	CLF	4	0
5	A	496	CFM	6	0
7	B	525	CLF	4	0
4	C	494	HCA	1	0
10	G	291	ADP	2	0
10	F	291	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

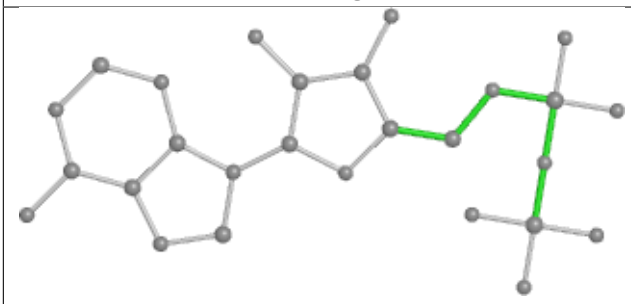
Ligand ADP E 291



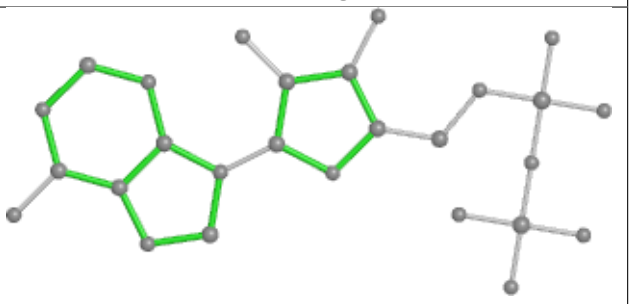
Bond lengths



Bond angles

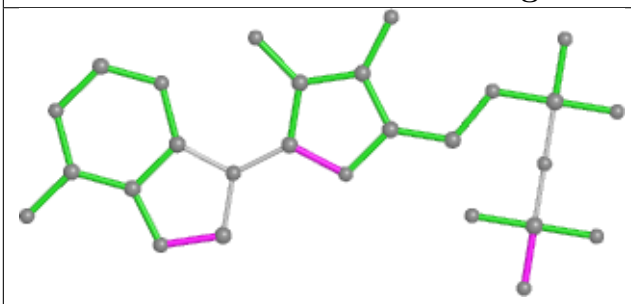


Torsions

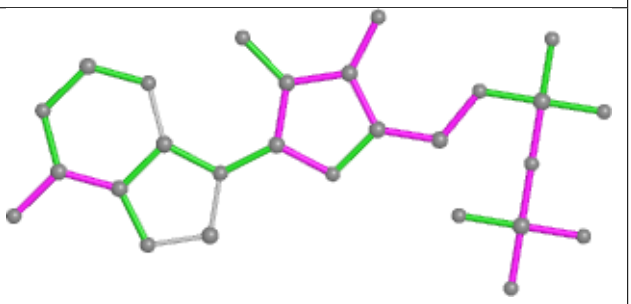


Rings

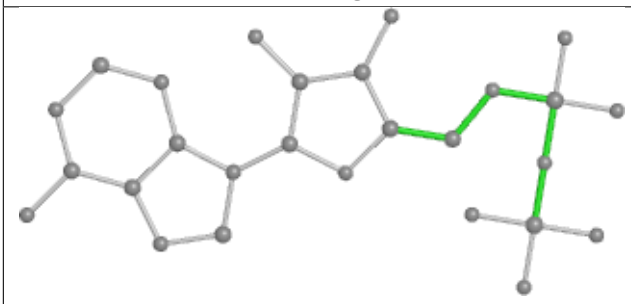
Ligand ADP H 291



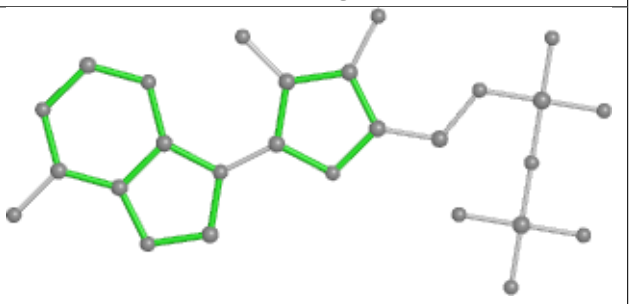
Bond lengths



Bond angles

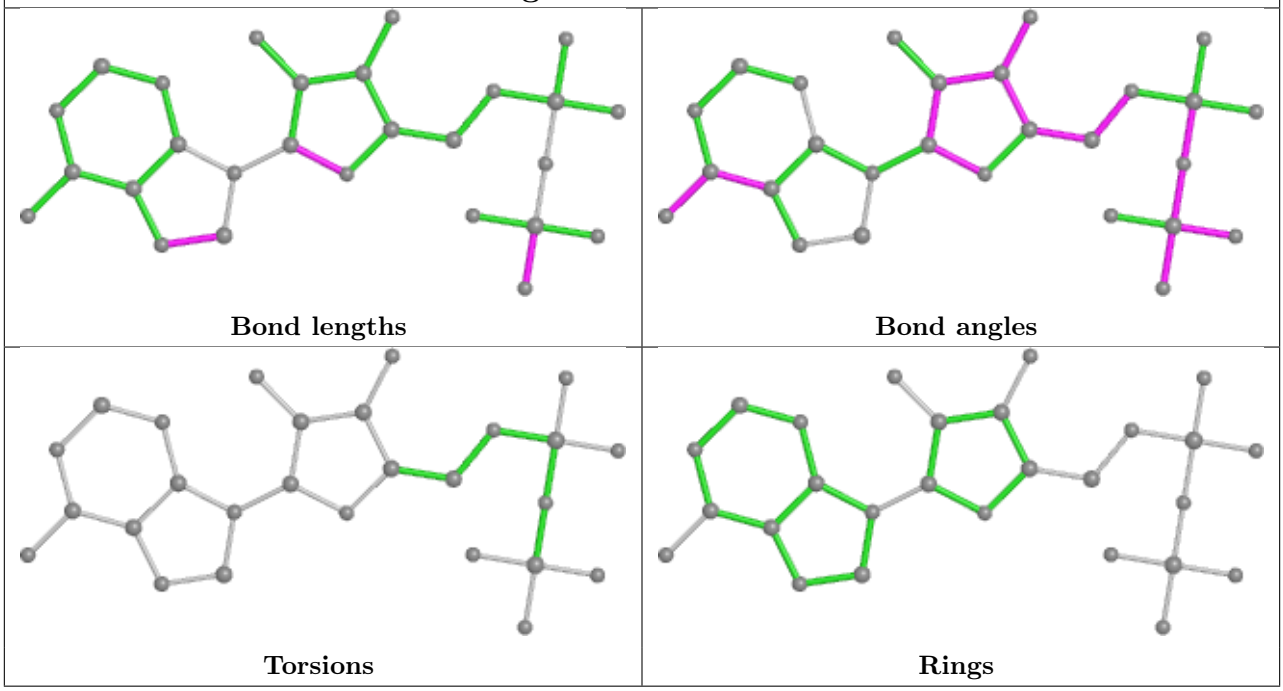


Torsions

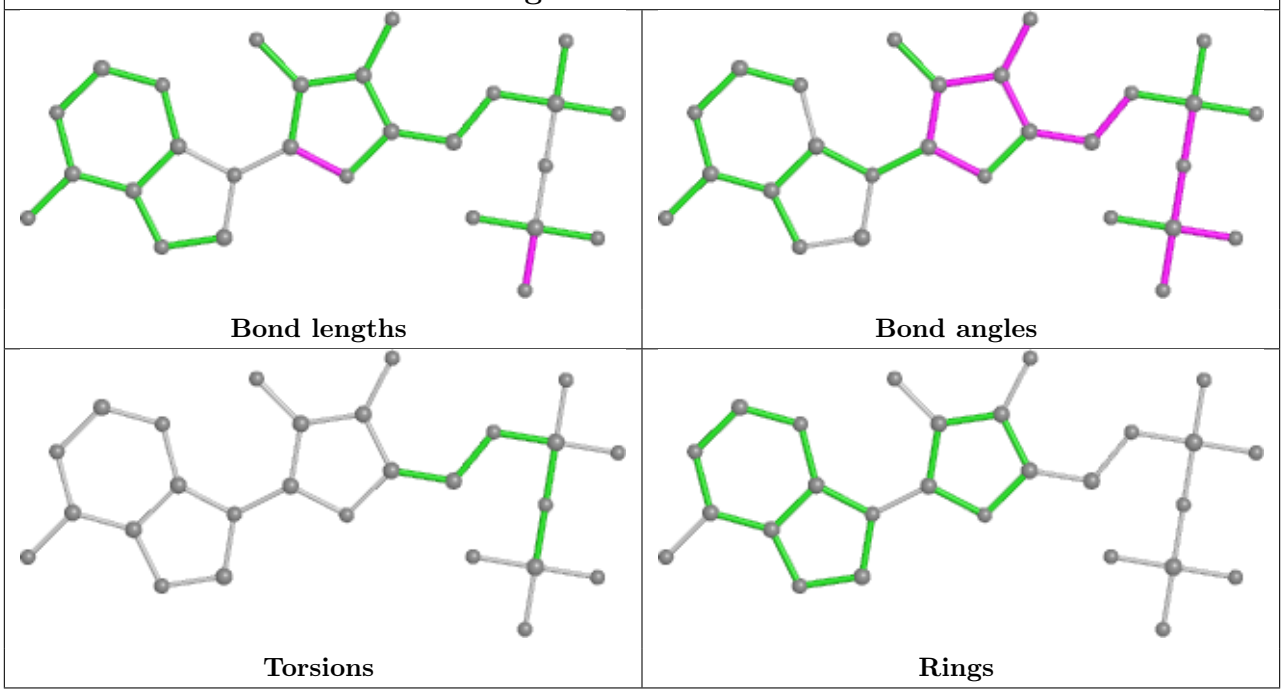


Rings

Ligand ADP G 291



Ligand ADP F 291



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.