



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:38 AM EDT

PDB ID : 1CP2 / pdb_00001cp2
Title : NITROGENASE IRON PROTEIN FROM CLOSTRIDIUM PASTEURIANUM
Authors : Schlessman, J.L.; Woo, D.; Joshua-Tor, L.; Howard, J.B.; Rees, D.C.
Deposited on : 1998-05-11
Resolution : 1.93 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

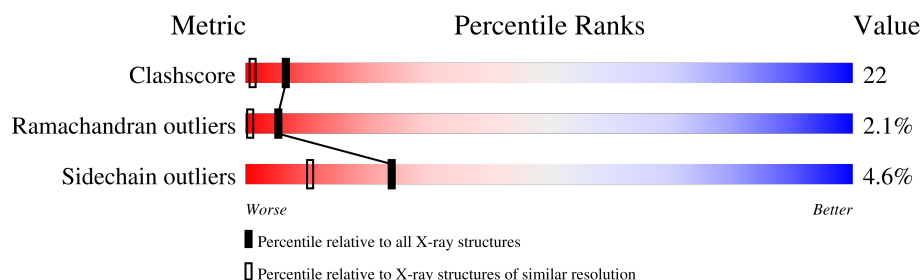
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	 62% 34% .
1	B	269	 58% 34% 7% .

2 Entry composition [i](#)

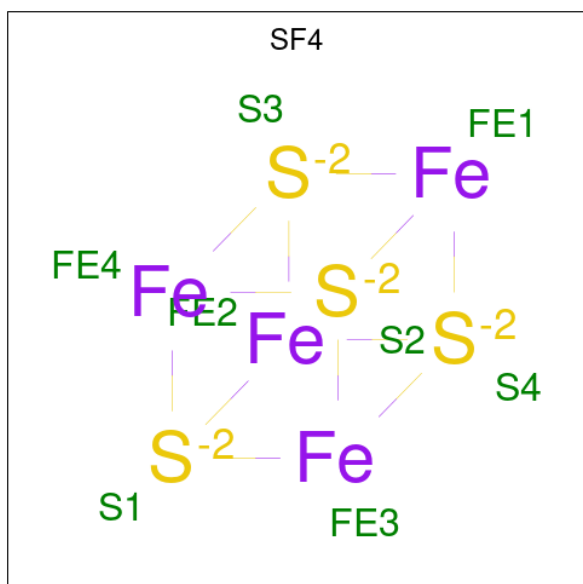
There are 3 unique types of molecules in this entry. The entry contains 4206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	83	0	0
			2040	1279	344	401	16			
1	B	269	Total	C	N	O	S	110	0	0
			2040	1279	344	401	16			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	56	Total	O	0	0
			56	56		

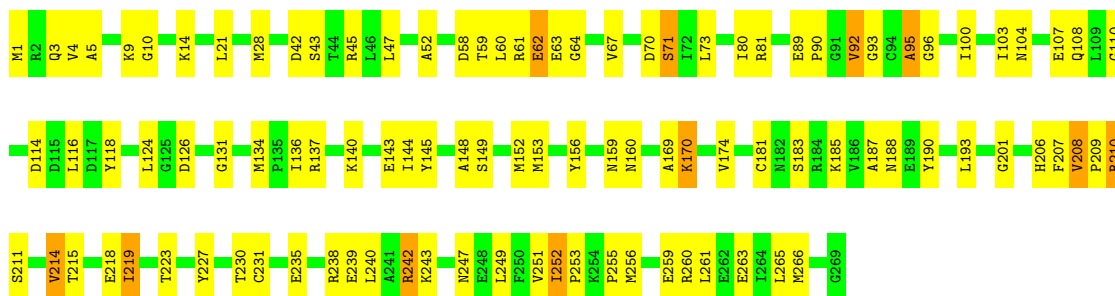
3 Residue-property plots

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.

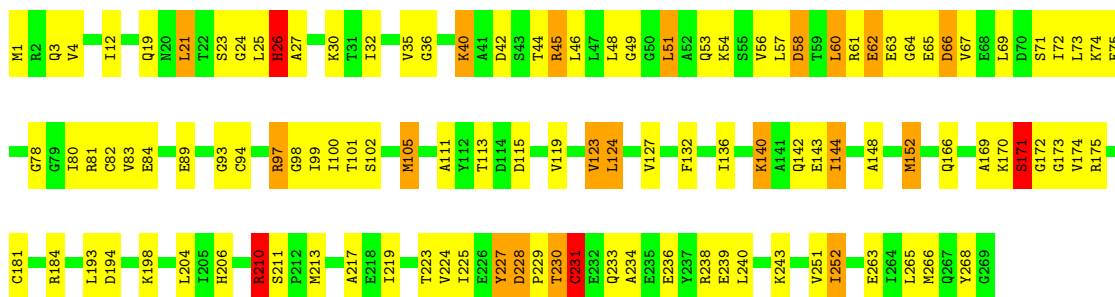
• Molecule 1: NITROGENASE IRON PROTEIN

Chain A: 



• Molecule 1: NITROGENASE IRON PROTEIN

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.60Å 75.87Å 53.55Å 90.00° 114.17° 90.00°	Depositor
Resolution (Å)	5.00 – 1.93	Depositor
% Data completeness (in resolution range)	98.8 (5.00-1.93)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4206	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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

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	1.02	2/2067 (0.1%)	1.33	21/2782 (0.8%)
1	B	1.09	6/2067 (0.3%)	1.34	24/2782 (0.9%)
All	All	1.06	8/4134 (0.2%)	1.34	45/5564 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ILE	CA-CB	6.54	1.61	1.53
1	B	12	ILE	CA-CB	6.20	1.61	1.54
1	A	266	MET	SD-CE	5.81	1.94	1.79
1	A	214	VAL	CA-CB	5.26	1.61	1.54
1	B	35	VAL	CA-CB	5.18	1.60	1.53
1	B	152	MET	SD-CE	5.06	1.92	1.79
1	B	127	VAL	CA-CB	5.05	1.60	1.54
1	B	21	LEU	CA-C	5.01	1.59	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ILE	N-CA-C	-15.50	93.46	107.56
1	B	230	THR	N-CA-C	-8.91	95.62	109.25
1	B	251	VAL	N-CA-C	8.28	121.90	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	THR	N-CA-C	-7.97	98.72	110.52
1	B	268	TYR	N-CA-C	7.55	123.54	113.72
1	B	40	LYS	N-CA-C	7.22	118.80	111.07
1	B	144	ILE	N-CA-C	6.93	118.58	108.53
1	B	123	VAL	N-CA-C	6.77	118.34	108.53
1	A	251	VAL	N-CA-C	6.75	118.66	108.80
1	B	219	ILE	N-CA-C	-6.74	103.65	111.00
1	B	231	CYS	N-CA-C	-6.54	96.88	110.80
1	A	208	VAL	CA-C-N	6.50	126.42	119.85
1	A	208	VAL	C-N-CA	6.50	126.42	119.85
1	B	211	SER	CA-C-N	-6.30	113.31	119.87
1	B	211	SER	C-N-CA	-6.30	113.31	119.87
1	B	58	ASP	N-CA-C	-6.18	103.48	111.02
1	A	230	THR	N-CA-C	6.17	120.81	113.28
1	A	95	ALA	N-CA-C	-6.14	104.50	111.07
1	B	26	HIS	N-CA-C	-6.10	104.54	111.07
1	A	149	SER	N-CA-C	-6.02	100.60	109.81
1	A	52	ALA	N-CA-C	-5.92	96.86	107.98
1	B	210	ARG	N-CA-C	-5.91	100.93	110.32
1	B	32	ILE	N-CA-C	5.89	118.36	108.81
1	A	219	ILE	CB-CA-C	-5.88	104.33	112.04
1	B	113	THR	N-CA-C	5.71	118.07	110.53
1	B	172	GLY	N-CA-C	-5.67	102.87	111.14
1	A	210	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	A	137	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	227	TYR	N-CA-C	5.40	118.08	111.82
1	A	45	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	72	ILE	N-CA-C	5.36	118.62	111.44
1	B	252	ILE	CA-C-N	5.34	125.28	119.78
1	B	252	ILE	C-N-CA	5.34	125.28	119.78
1	B	61	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	B	89	GLU	N-CA-C	-5.25	100.38	109.58
1	A	223	THR	N-CA-C	-5.22	102.80	110.52
1	A	43	SER	N-CA-C	5.21	119.49	113.18
1	A	61	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	45	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	252	ILE	N-CA-C	-5.10	97.87	108.88
1	A	201	GLY	N-CA-C	-5.03	108.29	115.64
1	A	118	TYR	N-CA-C	5.01	116.86	108.99
1	A	42	ASP	N-CA-C	-5.00	100.91	108.67
1	A	92	VAL	CA-C-N	-5.00	115.65	121.85
1	A	92	VAL	C-N-CA	-5.00	115.65	121.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Sidechain
1	A	210	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2040	0	2053	75	2
1	B	2040	0	2053	93	2
2	B	8	0	0	0	0
3	A	62	0	0	7	0
3	B	56	0	0	2	0
All	All	4206	0	4106	167	2

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 22.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:HE3	3:A:331:HOH:O	1.36	1.20
1:A:14:LYS:HB3	3:A:331:HOH:O	1.01	1.18
1:A:100:ILE:HD11	1:A:134:MET:HB3	1.24	1.13
1:B:93:GLY:HA2	1:B:97:ARG:HH22	1.31	0.94
1:B:60:LEU:HD12	1:B:67:VAL:HG21	1.50	0.93
1:A:188:ASN:HD21	1:A:190:TYR:HB2	1.39	0.87
1:A:131:GLY:O	1:A:134:MET:HG2	1.76	0.85
1:A:100:ILE:HD11	1:A:134:MET:CB	2.06	0.85
1:A:1:MET:HE2	1:A:116:LEU:HB2	1.60	0.83
1:B:144:ILE:HD11	1:B:174:VAL:CG1	2.12	0.79
1:B:94:CYS:HB3	1:B:97:ARG:HG3	1.64	0.78
1:B:97:ARG:O	1:B:100:ILE:HG13	1.85	0.77
1:B:93:GLY:HA2	1:B:97:ARG:NH2	2.00	0.77
1:B:19:GLN:HE22	1:B:46:LEU:H	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:CD1	1:B:67:VAL:HG21	2.15	0.75
1:B:144:ILE:HD12	1:B:175:ARG:O	1.86	0.75
1:A:214:VAL:O	1:A:218:GLU:HG3	1.86	0.74
1:B:26:HIS:CD2	1:B:78:GLY:HA3	2.22	0.74
1:B:67:VAL:HG11	1:B:105:MET:HE1	1.70	0.74
1:A:100:ILE:HG13	1:A:134:MET:HE3	1.70	0.73
1:B:54:LYS:HG2	1:B:58:ASP:HB2	1.71	0.72
1:B:97:ARG:HH11	1:B:97:ARG:HB2	1.53	0.72
1:A:159:ASN:HD21	1:A:256:MET:H	1.38	0.72
1:A:73:LEU:HD21	1:A:81:ARG:HB3	1.72	0.72
1:A:260:ARG:HH11	1:A:263:GLU:HB2	1.56	0.71
1:A:28:MET:SD	1:A:242:ARG:HG2	2.32	0.70
1:A:63:GLU:HB2	1:A:67:VAL:HG22	1.74	0.69
1:B:184:ARG:NH1	1:B:210:ARG:HE	1.90	0.69
1:B:26:HIS:NE2	1:B:78:GLY:HA3	2.09	0.68
1:A:21:LEU:HD13	1:A:240:LEU:HG	1.76	0.67
1:A:103:ILE:O	1:A:107:GLU:HG3	1.95	0.67
1:B:56:VAL:HG13	1:B:105:MET:CE	2.26	0.66
1:A:100:ILE:CD1	1:A:134:MET:HB3	2.16	0.66
1:A:96:GLY:O	1:A:100:ILE:HG12	1.95	0.66
1:A:64:GLY:O	1:A:67:VAL:HG23	1.97	0.64
1:A:131:GLY:O	1:A:134:MET:CG	2.46	0.64
1:B:42:ASP:HB3	1:B:45:ARG:HB2	1.79	0.63
1:B:1:MET:HE3	1:B:3:GLN:HE21	1.64	0.61
1:B:69:LEU:HD11	1:B:111:ALA:HB2	1.82	0.61
1:B:144:ILE:HD11	1:B:174:VAL:HG12	1.81	0.61
1:A:188:ASN:ND2	1:A:190:TYR:HB2	2.11	0.60
1:B:97:ARG:HH11	1:B:97:ARG:CB	2.15	0.60
1:B:56:VAL:HG13	1:B:105:MET:HE2	1.83	0.59
1:A:152:MET:HE1	1:A:261:LEU:HD23	1.84	0.58
1:B:225:ILE:HG13	3:B:327:HOH:O	2.01	0.58
1:B:60:LEU:HD12	1:B:67:VAL:CG2	2.31	0.58
1:B:67:VAL:HG11	1:B:105:MET:SD	2.44	0.58
1:B:67:VAL:HG11	1:B:105:MET:CE	2.33	0.58
1:B:73:LEU:HD12	1:B:82:CYS:O	2.05	0.57
1:A:124:LEU:HG	3:A:276:HOH:O	2.04	0.57
1:A:58:ASP:O	1:A:62:GLU:HG2	2.06	0.56
1:A:152:MET:HE3	1:A:156:TYR:HB2	1.87	0.56
1:B:144:ILE:HD11	1:B:174:VAL:HG13	1.86	0.56
1:A:14:LYS:CB	3:A:331:HOH:O	1.89	0.56
1:B:71:SER:O	1:B:74:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LYS:CG	1:B:58:ASP:CB	2.83	0.56
1:B:62:GLU:O	1:B:64:GLY:N	2.40	0.55
1:B:225:ILE:HA	1:B:234:ALA:HB1	1.88	0.55
1:A:60:LEU:HD23	1:A:67:VAL:HG21	1.88	0.55
1:B:193:LEU:HB3	1:B:204:LEU:HD13	1.89	0.55
1:B:230:THR:O	1:B:231:CYS:HB2	2.07	0.55
1:B:184:ARG:NH1	1:B:210:ARG:NE	2.54	0.54
1:B:1:MET:CE	1:B:3:GLN:HE21	2.19	0.54
1:B:54:LYS:HG2	1:B:58:ASP:CB	2.37	0.54
1:B:54:LYS:CG	1:B:58:ASP:HB2	2.36	0.54
1:B:239:GLU:CD	1:B:243:LYS:HE3	2.32	0.54
1:B:228:ASP:HB2	1:B:231:CYS:HB2	1.89	0.54
1:A:100:ILE:HG22	1:A:104:ASN:HD21	1.74	0.52
1:A:235:GLU:OE1	1:A:238:ARG:NH1	2.42	0.52
1:B:181:CYS:SG	1:B:193:LEU:HG	2.50	0.52
1:B:229:PRO:C	1:B:238:ARG:HH22	2.18	0.52
1:B:194:ASP:OD1	1:B:198:LYS:HE2	2.10	0.52
1:B:42:ASP:CB	1:B:45:ARG:HB2	2.40	0.51
1:A:215:THR:O	1:A:219:ILE:HG13	2.10	0.51
1:A:169:ALA:HB3	1:A:252:ILE:HG23	1.92	0.50
1:B:60:LEU:HD13	1:B:105:MET:HE2	1.93	0.50
1:A:89:GLU:O	1:A:92:VAL:O	2.29	0.50
1:B:229:PRO:HA	1:B:238:ARG:NH2	2.27	0.49
1:B:23:SER:HB3	1:B:225:ILE:HD12	1.94	0.49
1:B:217:ALA:HA	1:B:227:TYR:CE1	2.48	0.49
1:A:47:LEU:HD22	1:A:80:ILE:HD12	1.95	0.49
1:B:48:LEU:HB3	1:B:51:LEU:HB3	1.94	0.49
1:B:229:PRO:CA	1:B:238:ARG:HH22	2.26	0.48
1:A:4:VAL:HA	1:A:143:GLU:O	2.13	0.48
1:A:100:ILE:CG1	1:A:134:MET:HE3	2.39	0.48
1:B:166:GLN:O	1:B:166:GLN:HG2	2.13	0.48
1:B:21:LEU:HD13	1:B:240:LEU:HG	1.95	0.48
1:B:25:LEU:O	1:B:30:LYS:HB2	2.14	0.48
1:A:152:MET:CE	1:A:156:TYR:HB2	2.44	0.47
1:A:1:MET:HE2	1:A:116:LEU:CB	2.38	0.47
1:B:142:GLN:OE1	1:B:173:GLY:HA3	2.13	0.47
1:B:36:GLY:HA3	1:B:84:GLU:OE1	2.15	0.47
1:A:206:HIS:HB3	1:A:240:LEU:HD13	1.95	0.47
1:A:231:CYS:HB2	3:A:297:HOH:O	2.14	0.47
1:B:136:ILE:HG23	1:B:174:VAL:HG21	1.96	0.47
1:B:206:HIS:HB3	1:B:240:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HG22	1:A:104:ASN:ND2	2.29	0.47
1:A:148:ALA:O	1:A:181:CYS:HA	2.14	0.47
1:B:42:ASP:CG	1:B:45:ARG:HB2	2.40	0.47
1:B:233:GLN:O	1:B:236:GLU:HB2	2.14	0.47
1:B:3:GLN:HB3	1:B:140:LYS:O	2.15	0.46
1:B:263:GLU:O	1:B:266:MET:HB3	2.14	0.46
1:B:124:LEU:HD22	1:B:132:PHE:CE2	2.50	0.46
1:A:238:ARG:O	1:A:242:ARG:HG3	2.15	0.46
1:B:227:TYR:HD2	1:B:228:ASP:OD1	1.99	0.46
1:A:188:ASN:ND2	1:A:188:ASN:C	2.72	0.46
1:B:73:LEU:HA	1:B:82:CYS:O	2.15	0.46
1:A:108:GLN:O	1:A:108:GLN:HG2	2.16	0.45
1:A:185:LYS:CE	1:A:187:ALA:HB3	2.46	0.45
1:B:213:MET:SD	1:B:233:GLN:HB2	2.57	0.45
1:A:3:GLN:HB3	1:A:140:LYS:O	2.17	0.45
1:B:119:VAL:HG11	3:B:298:HOH:O	2.17	0.45
1:A:100:ILE:HG13	1:A:134:MET:CE	2.43	0.44
1:A:239:GLU:O	1:A:243:LYS:HD2	2.18	0.44
1:B:100:ILE:HD12	1:B:101:THR:N	2.33	0.44
1:A:188:ASN:C	1:A:188:ASN:HD22	2.26	0.44
1:B:213:MET:SD	1:B:231:CYS:SG	3.15	0.44
1:B:54:LYS:CG	1:B:58:ASP:HB3	2.48	0.44
1:A:153:MET:HE1	1:B:40:LYS:O	2.17	0.44
1:B:224:VAL:O	1:B:225:ILE:C	2.59	0.44
1:A:60:LEU:O	1:A:64:GLY:HA2	2.18	0.43
1:B:169:ALA:HB1	1:B:252:ILE:HG12	1.99	0.43
1:A:253:PRO:O	1:A:255:PRO:HD3	2.18	0.43
1:B:152:MET:HG2	1:B:265:LEU:HD13	1.99	0.43
1:A:256:MET:HE2	1:A:256:MET:HB3	1.90	0.43
1:B:24:GLY:O	1:B:27:ALA:HB3	2.19	0.43
1:B:239:GLU:O	1:B:243:LYS:HG3	2.18	0.43
1:A:59:THR:HG21	1:A:71:SER:OG	2.19	0.43
1:A:243:LYS:O	1:A:247:ASN:HB2	2.19	0.43
1:A:152:MET:HE1	1:A:261:LEU:CD2	2.48	0.43
1:A:249:LEU:HA	1:A:249:LEU:HD12	1.70	0.43
1:B:62:GLU:C	1:B:64:GLY:H	2.26	0.43
1:A:5:ALA:HB3	1:A:144:ILE:HD13	2.01	0.43
1:A:14:LYS:CE	3:A:331:HOH:O	2.11	0.43
1:A:181:CYS:HB2	1:A:193:LEU:HG	2.01	0.43
1:A:208:VAL:HA	1:A:209:PRO:HD3	1.78	0.43
1:A:107:GLU:HG3	1:A:107:GLU:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:O	1:B:231:CYS:CB	2.67	0.42
1:B:98:GLY:O	1:B:99:ILE:C	2.61	0.42
1:B:229:PRO:CA	1:B:238:ARG:NH2	2.83	0.42
1:A:183:SER:HB2	1:A:207:PHE:CZ	2.55	0.42
1:A:211:SER:O	1:A:214:VAL:HG22	2.19	0.42
1:A:1:MET:CE	1:A:116:LEU:HD12	2.50	0.42
1:A:124:LEU:HD11	1:A:126:ASP:OD2	2.20	0.42
1:B:56:VAL:HG11	1:B:102:SER:HA	2.02	0.42
1:B:229:PRO:HA	1:B:238:ARG:HH22	1.84	0.42
1:A:260:ARG:NH1	1:A:263:GLU:HB2	2.30	0.42
1:A:136:ILE:HG23	1:A:174:VAL:HG11	2.02	0.42
1:B:170:LYS:O	1:B:171:SER:CB	2.68	0.42
1:B:124:LEU:HD22	1:B:132:PHE:CD2	2.55	0.41
1:A:95:ALA:O	1:A:96:GLY:C	2.63	0.41
1:A:206:HIS:ND1	1:A:243:LYS:NZ	2.60	0.41
1:B:1:MET:HE2	1:B:1:MET:HB3	1.79	0.41
1:B:4:VAL:HA	1:B:143:GLU:O	2.20	0.41
1:B:148:ALA:O	1:B:181:CYS:HA	2.20	0.41
1:B:44:THR:OG1	1:B:53:GLN:NE2	2.53	0.41
1:A:96:GLY:CA	1:A:134:MET:HG3	2.50	0.41
1:B:73:LEU:HD11	1:B:81:ARG:CB	2.50	0.41
1:A:9:LYS:NZ	1:A:10:GLY:O	2.53	0.41
1:A:110:GLY:HA2	3:A:324:HOH:O	2.21	0.41
1:B:65:GLU:O	1:B:67:VAL:N	2.50	0.41
1:B:19:GLN:NE2	1:B:44:THR:HA	2.36	0.40
1:B:81:ARG:NH2	1:B:115:ASP:OD2	2.49	0.40
1:B:100:ILE:HD12	1:B:100:ILE:C	2.46	0.40
1:B:227:TYR:O	1:B:229:PRO:HD3	2.21	0.40
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.80	0.40
1:A:92:VAL:HG12	1:A:93:GLY:N	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:CE	1:B:266:MET:CE[1_554]	1.45	0.75
1:A:170:LYS:NZ	1:B:266:MET:CE[1_554]	1.98	0.22

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	267/269 (99%)	256 (96%)	8 (3%)	3 (1%)	11	4
1	B	267/269 (99%)	245 (92%)	14 (5%)	8 (3%)	3	0
All	All	534/538 (99%)	501 (94%)	22 (4%)	11 (2%)	5	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	B	63	GLU
1	B	171	SER
1	B	227	TYR
1	A	114	ASP
1	B	62	GLU
1	B	140	LYS
1	B	231	CYS
1	A	70	ASP
1	B	66	ASP
1	B	49	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	217/217 (100%)	211 (97%)	6 (3%)	38	25
1	B	217/217 (100%)	203 (94%)	14 (6%)	15	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	434/434 (100%)	414 (95%)	20 (5%)	24	10

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	71	SER
1	A	90	PRO
1	A	160	ASN
1	A	242	ARG
1	A	259	GLU
1	B	26	HIS
1	B	51	LEU
1	B	57	LEU
1	B	60	LEU
1	B	66	ASP
1	B	75	GLU
1	B	83	VAL
1	B	97	ARG
1	B	105	MET
1	B	123	VAL
1	B	124	LEU
1	B	171	SER
1	B	210	ARG
1	B	228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	108	GLN
1	A	159	ASN
1	A	182	ASN
1	A	188	ASN
1	A	233	GLN
1	A	258	GLN
1	B	3	GLN
1	B	19	GLN
1	B	53	GLN
1	B	104	ASN
1	B	166	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	B	290	1,3	0,12,12	-	-	-		

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
2	SF4	B	290	1,3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.