



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:32 AM UTC

PDB ID : 1XDB / pdb_00001xdb
Title : Crystal Structure of the Nitrogenase Fe protein Asp129Glu
Authors : Jang, S.B.; Jeong, M.S.; Seefeldt, L.C.; Peters, J.W.
Deposited on : 2004-09-05
Resolution : 2.80 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

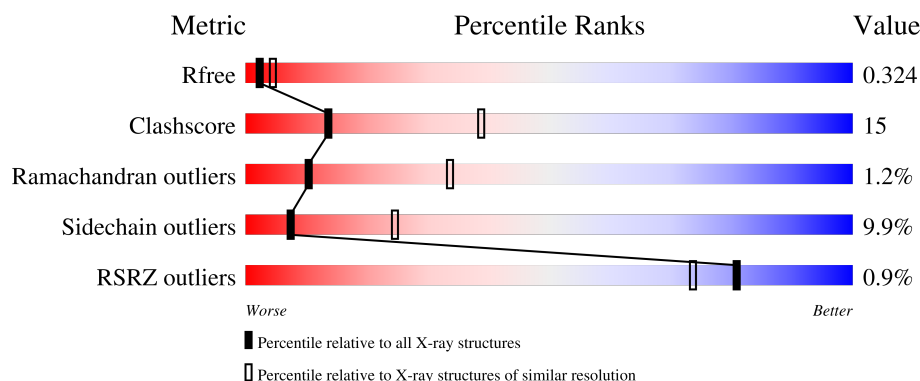
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	289	% 57% 35% 7% .
1	B	289	% 56% 32% 10% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4384 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.

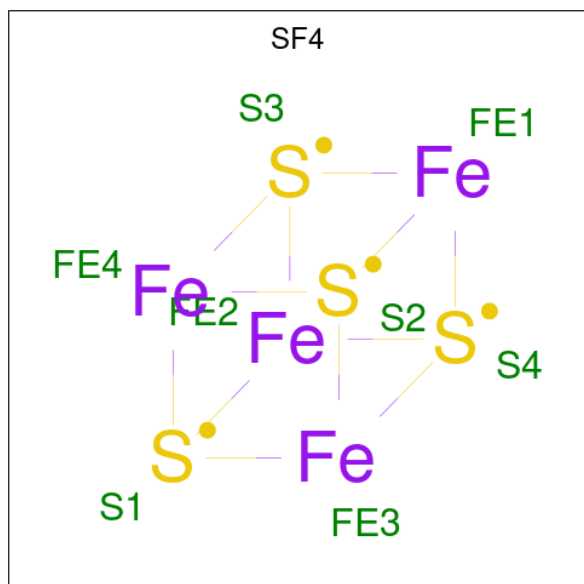
- Molecule 1 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2188	1365	369	433	21			
1	B	289	Total	C	N	O	S	0	0	0
			2188	1365	369	433	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	GLU	ASP	engineered mutation	UNP P00459
B	129	GLU	ASP	engineered mutation	UNP P00459

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

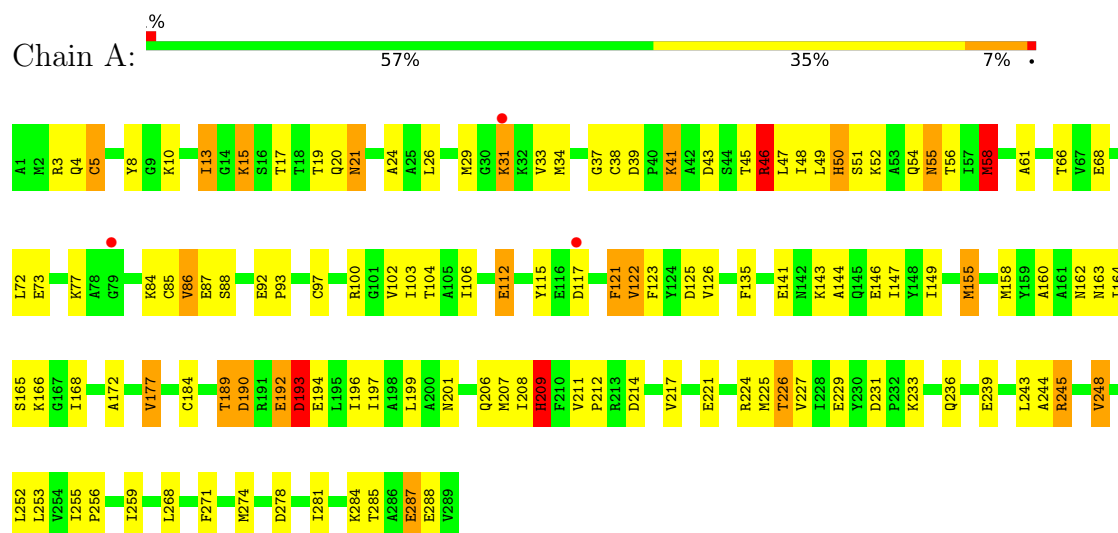


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

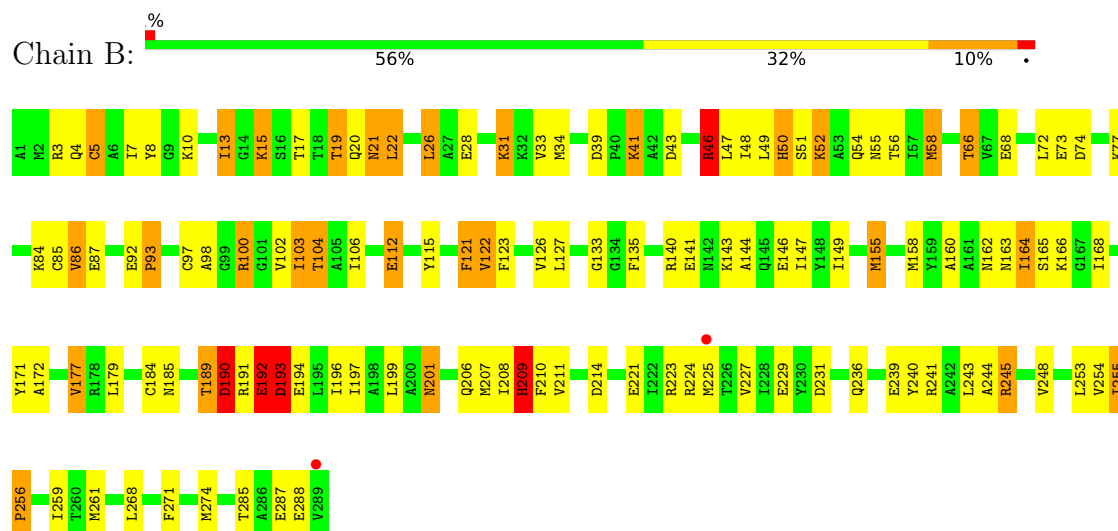
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nitrogenase iron protein 1



• Molecule 1: Nitrogenase iron protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.57Å 92.14Å 63.93Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (20.00-2.80) 87.4 (20.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.79Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , 0.299 0.246 , 0.324	Depositor DCC
R_{free} test set	683 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.99	2/2212 (0.1%)	1.84	40/2978 (1.3%)
1	B	0.99	3/2212 (0.1%)	1.85	48/2978 (1.6%)
All	All	0.99	5/4424 (0.1%)	1.85	88/5956 (1.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	50	HIS	CD2-NE2	-6.78	1.30	1.37
1	B	50	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	209	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	50	HIS	CG-ND1	-5.00	1.32	1.38

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ARG	CD-NE-CZ	14.04	144.05	124.40
1	A	245	ARG	CD-NE-CZ	14.03	144.04	124.40
1	B	245	ARG	CD-NE-CZ	13.92	143.89	124.40
1	B	100	ARG	NE-CZ-NH2	13.89	131.70	119.20
1	A	100	ARG	CD-NE-CZ	13.53	143.34	124.40
1	B	245	ARG	NE-CZ-NH2	12.77	130.69	119.20
1	A	245	ARG	NE-CZ-NH1	11.72	133.22	121.50
1	B	100	ARG	NE-CZ-NH1	-11.50	110.00	121.50
1	A	100	ARG	NE-CZ-NH1	10.06	131.56	121.50
1	A	100	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	B	193	ASP	CA-CB-CG	9.79	122.39	112.60
1	A	245	ARG	NE-CZ-NH2	-9.27	110.86	119.20
1	B	245	ARG	NE-CZ-NH1	-9.15	112.35	121.50
1	A	193	ASP	CA-CB-CG	8.66	121.26	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PHE	N-CA-C	7.99	122.64	109.06
1	A	13	ILE	N-CA-C	-7.95	105.12	112.43
1	B	13	ILE	N-CA-C	-7.93	105.14	112.43
1	B	121	PHE	N-CA-C	7.67	122.09	109.06
1	B	192	GLU	N-CA-C	7.55	120.39	111.71
1	B	74	ASP	N-CA-C	7.07	119.06	111.36
1	A	31	LYS	N-CA-C	7.06	120.45	110.50
1	A	192	GLU	N-CA-C	6.99	119.75	111.71
1	B	102	VAL	CA-C-O	-6.93	113.50	120.85
1	B	189	THR	CA-CB-OG1	-6.92	99.22	109.60
1	B	211	VAL	CA-C-N	6.90	126.66	119.76
1	B	211	VAL	C-N-CA	6.90	126.66	119.76
1	A	231	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	31	LYS	N-CA-C	6.82	120.11	110.50
1	B	231	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	214	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	217	VAL	N-CA-C	-6.63	104.06	110.42
1	A	256	PRO	N-CA-C	6.61	120.47	111.22
1	B	201	ASN	CA-CB-CG	6.31	118.91	112.60
1	A	189	THR	CA-CB-OG1	-6.23	100.25	109.60
1	B	135	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	104	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	211	VAL	CA-C-N	6.08	125.84	119.76
1	A	211	VAL	C-N-CA	6.08	125.84	119.76
1	A	86	VAL	CB-CA-C	-6.05	100.24	110.71
1	A	221	GLU	CA-CB-CG	6.00	126.10	114.10
1	B	221	GLU	CA-CB-CG	5.94	125.98	114.10
1	B	214	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	211	VAL	N-CA-C	5.87	113.36	107.55
1	B	97	CYS	N-CA-C	-5.84	100.14	109.96
1	B	98	ALA	O-C-N	5.77	128.24	122.12
1	A	135	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	102	VAL	CA-C-O	-5.75	114.66	121.05
1	A	5	CYS	N-CA-C	5.75	118.92	109.72
1	B	19	THR	CA-CB-OG1	-5.74	101.00	109.60
1	B	22	LEU	N-CA-C	-5.72	104.96	111.14
1	A	190	ASP	N-CA-C	5.72	122.99	110.80
1	A	248	VAL	CA-C-O	5.72	126.90	120.95
1	B	5	CYS	N-CA-C	5.65	118.76	109.72
1	B	190	ASP	N-CA-C	5.64	122.82	110.80
1	B	92	GLU	CA-C-N	5.62	126.86	119.84
1	B	92	GLU	C-N-CA	5.62	126.86	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	CYS	N-CA-C	-5.53	100.67	109.96
1	B	86	VAL	CB-CA-C	-5.50	101.88	110.69
1	B	254	VAL	N-CA-C	5.46	116.77	108.80
1	B	46	ARG	N-CA-C	5.45	122.42	110.80
1	B	185	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	58	MET	CA-CB-CG	-5.43	103.24	114.10
1	B	133	GLY	CA-C-N	5.37	125.90	119.94
1	B	133	GLY	C-N-CA	5.37	125.90	119.94
1	B	100	ARG	CB-CG-CD	-5.37	98.96	111.30
1	B	256	PRO	N-CA-C	5.36	118.72	111.22
1	A	287	GLU	O-C-N	5.35	127.81	122.03
1	A	61	ALA	N-CA-C	-5.32	105.56	111.36
1	B	103	ILE	N-CA-CB	5.29	116.74	110.55
1	A	43	ASP	N-CA-C	5.25	119.31	113.01
1	A	103	ILE	N-CA-CB	5.25	116.69	110.55
1	A	43	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	210	PHE	CA-C-O	5.21	125.77	120.24
1	B	255	ILE	N-CA-C	-5.20	101.95	107.77
1	B	127	LEU	CA-C-O	5.17	126.75	120.81
1	A	92	GLU	CA-C-N	5.16	126.29	119.84
1	A	92	GLU	C-N-CA	5.16	126.29	119.84
1	B	189	THR	CA-CB-CG2	5.15	119.25	110.50
1	A	117	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	26	LEU	N-CA-C	5.08	117.72	111.82
1	B	43	ASP	N-CA-C	5.08	119.11	113.01
1	A	209	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	19	THR	CA-CB-OG1	-5.05	102.02	109.60
1	A	212	PRO	CA-C-O	-5.05	115.25	121.31
1	A	55	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	66	THR	CA-CB-OG1	-5.03	102.05	109.60
1	A	103	ILE	CB-CA-C	-5.02	105.55	111.97
1	B	164	ILE	O-C-N	5.01	126.95	121.94

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	2188	0	2199	63	0
1	B	2188	0	2200	69	0
2	A	8	0	0	0	0
All	All	4384	0	4399	128	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 15.

All (128) 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:B:209:HIS:HB2	1:B:243:LEU:HD13	1.47	0.93
1:A:209:HIS:HB2	1:A:243:LEU:HD13	1.51	0.89
1:B:15:LYS:HE3	1:B:126:VAL:O	1.90	0.71
1:A:33:VAL:HG22	1:A:121:PHE:HB2	1.75	0.69
1:A:20:GLN:HE22	1:A:47:LEU:H	1.42	0.67
1:B:4:GLN:HA	1:B:122:VAL:HG23	1.75	0.67
1:A:4:GLN:HA	1:A:122:VAL:HG23	1.76	0.67
1:A:15:LYS:HE3	1:A:126:VAL:O	1.95	0.65
1:B:172:ALA:HB1	1:B:255:ILE:HD13	1.80	0.62
1:B:33:VAL:HG22	1:B:121:PHE:HB2	1.81	0.62
1:B:20:GLN:HE22	1:B:47:LEU:H	1.48	0.60
1:B:8:TYR:HB3	1:B:164:ILE:HD13	1.83	0.60
1:A:66:THR:HG23	1:A:68:GLU:H	1.67	0.59
1:A:41:LYS:HZ3	1:B:261:MET:HE3	1.68	0.58
1:A:3:ARG:HH12	1:A:248:VAL:HA	1.69	0.58
1:A:172:ALA:HB1	1:A:255:ILE:HD13	1.86	0.56
1:B:162:ASN:HD21	1:B:259:ILE:H	1.53	0.56
1:A:162:ASN:HD21	1:A:259:ILE:H	1.54	0.56
1:B:268:LEU:HB3	1:B:274:MET:HB2	1.88	0.55
1:B:194:GLU:HG3	1:B:271:PHE:HE2	1.72	0.55
1:B:3:ARG:HH12	1:B:248:VAL:HA	1.72	0.55
1:B:146:GLU:HG2	1:B:253:LEU:HD11	1.90	0.53
1:B:106:ILE:HG21	1:B:143:LYS:HG2	1.91	0.53
1:A:17:THR:O	1:A:21:ASN:HB2	2.09	0.52
1:B:194:GLU:HG3	1:B:271:PHE:CE2	2.44	0.52
1:A:165:SER:HA	1:A:168:ILE:HG12	1.92	0.52
1:A:285:THR:HG23	1:A:287:GLU:HB2	1.91	0.52
1:A:106:ILE:HG21	1:A:143:LYS:HG2	1.91	0.52
1:A:268:LEU:HB3	1:A:274:MET:HB2	1.91	0.52
1:B:115:TYR:HE2	1:B:122:VAL:HG11	1.75	0.52
1:A:8:TYR:HB3	1:A:164:ILE:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ASN:HD21	1:B:227:VAL:H	1.57	0.51
1:B:193:ASP:O	1:B:197:ILE:HG13	2.09	0.51
1:A:196:ILE:HG22	1:A:207:MET:HG3	1.93	0.51
1:A:184:CYS:HB2	1:A:196:ILE:HG21	1.91	0.51
1:A:285:THR:HG22	1:A:288:GLU:OE1	2.11	0.51
1:B:66:THR:HG23	1:B:68:GLU:H	1.75	0.51
1:A:20:GLN:HE21	1:A:48:ILE:HG12	1.76	0.50
1:A:193:ASP:O	1:A:197:ILE:HG13	2.11	0.50
1:B:196:ILE:HG22	1:B:207:MET:HG3	1.93	0.50
1:B:49:LEU:HD11	1:B:77:LYS:HB3	1.93	0.50
1:B:50:HIS:HA	1:B:224:ARG:O	2.11	0.50
1:B:225:MET:HE3	1:B:229:GLU:HG2	1.93	0.50
1:A:34:MET:HA	1:A:84:LYS:O	2.11	0.50
1:B:162:ASN:O	1:B:165:SER:HB2	2.12	0.50
1:B:165:SER:HA	1:B:168:ILE:HG12	1.94	0.49
1:B:41:LYS:NZ	1:B:46:ARG:HH22	2.11	0.49
1:A:155:MET:C	1:A:155:MET:SD	2.95	0.49
1:B:58:MET:HE1	1:B:104:THR:HG21	1.94	0.49
1:A:93:PRO:HG3	1:B:166:LYS:HD3	1.95	0.49
1:B:184:CYS:HB2	1:B:196:ILE:HG21	1.95	0.49
1:B:285:THR:HG23	1:B:287:GLU:HB2	1.96	0.48
1:A:162:ASN:O	1:A:165:SER:HB2	2.14	0.48
1:B:5:CYS:O	1:B:123:PHE:HA	2.14	0.48
1:A:10:LYS:O	1:A:13:ILE:HG12	2.14	0.48
1:B:209:HIS:CB	1:B:243:LEU:HD13	2.32	0.47
1:B:179:LEU:HD23	1:B:256:PRO:HB3	1.96	0.47
1:A:5:CYS:O	1:A:123:PHE:HA	2.14	0.47
1:B:22:LEU:HD13	1:B:243:LEU:HG	1.97	0.47
1:A:49:LEU:HD11	1:A:77:LYS:HB3	1.97	0.47
1:A:194:GLU:HG3	1:A:271:PHE:HE2	1.80	0.47
1:A:160:ALA:O	1:A:164:ILE:HG13	2.15	0.47
1:B:158:MET:HE2	1:B:199:LEU:HD22	1.96	0.47
1:B:160:ALA:O	1:B:164:ILE:HG13	2.15	0.46
1:B:236:GLN:O	1:B:239:GLU:HB2	2.15	0.46
1:B:72:LEU:HB2	1:B:112:GLU:HG2	1.97	0.46
1:B:285:THR:HG22	1:B:288:GLU:OE1	2.15	0.46
1:A:46:ARG:HG3	1:A:51:SER:O	2.16	0.46
1:A:8:TYR:O	1:A:149:ILE:HA	2.15	0.46
1:A:21:ASN:HD21	1:A:227:VAL:H	1.64	0.46
1:B:46:ARG:HG3	1:B:51:SER:O	2.15	0.46
1:B:191:ARG:O	1:B:194:GLU:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:THR:O	1:B:21:ASN:HB2	2.16	0.45
1:B:47:LEU:O	1:B:225:MET:HA	2.16	0.45
1:B:28:GLU:OE2	1:B:241:ARG:HD3	2.16	0.45
1:B:56:THR:HG22	1:B:87:GLU:HB3	1.99	0.45
1:B:146:GLU:HG2	1:B:253:LEU:CD1	2.46	0.45
1:B:54:GLN:HG2	1:B:55:ASN:N	2.32	0.45
1:B:46:ARG:HD2	1:B:52:LYS:O	2.16	0.45
1:A:72:LEU:HB2	1:A:112:GLU:HG2	1.99	0.45
1:A:194:GLU:HG3	1:A:271:PHE:CE2	2.52	0.44
1:A:233:LYS:HE3	1:A:233:LYS:HB2	1.79	0.44
1:B:3:ARG:HB2	1:B:121:PHE:CE2	2.52	0.44
1:B:21:ASN:HB3	1:B:240:TYR:CD1	2.52	0.44
1:A:24:ALA:HB2	1:A:226:THR:HG21	1.98	0.44
1:A:225:MET:HE3	1:A:229:GLU:HG2	1.99	0.44
1:B:8:TYR:O	1:B:149:ILE:HA	2.17	0.44
1:B:34:MET:HA	1:B:84:LYS:O	2.18	0.44
1:B:100:ARG:HA	1:B:103:ILE:HG12	1.99	0.44
1:A:37:GLY:O	1:A:88:SER:HB3	2.18	0.44
1:B:144:ALA:O	1:B:177:VAL:HG13	2.17	0.44
1:B:155:MET:SD	1:B:155:MET:C	3.00	0.44
1:A:236:GLN:O	1:A:239:GLU:HB2	2.18	0.43
1:B:20:GLN:HE21	1:B:48:ILE:HG12	1.82	0.43
1:A:284:LYS:O	1:B:223:ARG:HD3	2.18	0.43
1:A:38:CYS:HB2	1:A:125:ASP:O	2.18	0.43
1:B:26:LEU:O	1:B:31:LYS:HB2	2.18	0.43
1:A:46:ARG:HD2	1:A:52:LYS:O	2.18	0.43
1:B:140:ARG:HG3	1:B:171:TYR:CE1	2.54	0.43
1:A:26:LEU:HA	1:A:29:MET:HG2	2.01	0.43
1:A:20:GLN:HE22	1:A:47:LEU:N	2.13	0.42
1:A:50:HIS:HA	1:A:224:ARG:O	2.20	0.42
1:A:54:GLN:HG2	1:A:55:ASN:N	2.33	0.42
1:B:20:GLN:HE22	1:B:47:LEU:N	2.13	0.42
1:A:147:ILE:HG21	1:A:168:ILE:HD11	2.01	0.42
1:A:41:LYS:NZ	1:A:46:ARG:HH22	2.17	0.42
1:B:285:THR:HG23	1:B:288:GLU:HG3	2.02	0.42
1:A:285:THR:HG23	1:A:288:GLU:HG3	2.02	0.42
1:A:158:MET:HE2	1:A:199:LEU:HD22	2.02	0.42
1:A:144:ALA:O	1:A:177:VAL:HG13	2.19	0.42
1:A:146:GLU:HG2	1:A:253:LEU:HD11	2.02	0.41
1:A:26:LEU:HD13	1:A:244:ALA:HB1	2.02	0.41
1:A:166:LYS:HD3	1:B:93:PRO:HG3	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:N	1:A:31:LYS:HD2	2.34	0.41
1:B:149:ILE:HG23	1:B:164:ILE:HD12	2.03	0.41
1:B:7:ILE:HG21	1:B:19:THR:OG1	2.20	0.41
1:B:10:LYS:O	1:B:13:ILE:HG12	2.21	0.41
1:A:58:MET:HE1	1:A:104:THR:HG21	2.02	0.41
1:A:278:ASP:HB3	1:A:281:ILE:HG12	2.03	0.41
1:A:115:TYR:HE2	1:A:122:VAL:HG11	1.84	0.41
1:A:45:THR:CG2	1:A:85:CYS:HB3	2.50	0.41
1:B:49:LEU:HD21	1:B:85:CYS:HB2	2.01	0.41
1:B:26:LEU:HD13	1:B:244:ALA:HB1	2.03	0.41
1:B:192:GLU:O	1:B:196:ILE:HG12	2.21	0.40
1:A:3:ARG:HB2	1:A:121:PHE:CE2	2.56	0.40
1:A:209:HIS:CB	1:A:243:LEU:HD13	2.36	0.40
1:B:147:ILE:HG21	1:B:168:ILE:HD11	2.02	0.40
1:A:56:THR:HG22	1:A:87:GLU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/289 (99%)	263 (92%)	21 (7%)	3 (1%)	12	38
1	B	287/289 (99%)	262 (91%)	21 (7%)	4 (1%)	9	30
All	All	574/578 (99%)	525 (92%)	42 (7%)	7 (1%)	10	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	ILE
1	B	46	ARG
1	A	46	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	252	LEU
1	A	208	ILE
1	B	190	ASP
1	B	93	PRO

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	233/233 (100%)	210 (90%)	23 (10%)	7	24
1	B	233/233 (100%)	210 (90%)	23 (10%)	7	24
All	All	466/466 (100%)	420 (90%)	46 (10%)	7	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	21	ASN
1	A	39	ASP
1	A	41	LYS
1	A	46	ARG
1	A	58	MET
1	A	73	GLU
1	A	86	VAL
1	A	112	GLU
1	A	122	VAL
1	A	141	GLU
1	A	155	MET
1	A	163	ASN
1	A	177	VAL
1	A	189	THR
1	A	190	ASP
1	A	192	GLU
1	A	193	ASP
1	A	201	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	GLN
1	A	209	HIS
1	A	226	THR
1	A	245	ARG
1	B	15	LYS
1	B	21	ASN
1	B	39	ASP
1	B	41	LYS
1	B	46	ARG
1	B	52	LYS
1	B	58	MET
1	B	73	GLU
1	B	86	VAL
1	B	112	GLU
1	B	122	VAL
1	B	141	GLU
1	B	155	MET
1	B	163	ASN
1	B	177	VAL
1	B	189	THR
1	B	190	ASP
1	B	192	GLU
1	B	193	ASP
1	B	201	ASN
1	B	206	GLN
1	B	209	HIS
1	B	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN
1	A	107	ASN
1	A	162	ASN
1	A	218	GLN
1	B	4	GLN
1	B	20	GLN
1	B	21	ASN
1	B	54	GLN
1	B	107	ASN
1	B	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	ASN
1	B	206	GLN
1	B	218	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	A	290	1	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	A	290	1	-	-	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/289 (100%)	0.01	3 (1%) 79 72	33, 74, 98, 100	0
1	B	289/289 (100%)	0.11	2 (0%) 84 77	39, 80, 99, 100	0
All	All	578/578 (100%)	0.06	5 (0%) 81 74	33, 77, 99, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	LYS	2.6
1	B	289	VAL	2.6
1	B	225	MET	2.5
1	A	79	GLY	2.1
1	A	117	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	A	290	8/8	0.99	0.02	19,27,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.