



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 10:15 PM EDT

PDB ID : 1XDB  
Title : Crystal Structure of the Nitrogenase Fe protein Asp129Glu  
Authors : Jang, S.B.; Jeong, M.S.; Seefeldt, L.C.; Peters, J.W.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

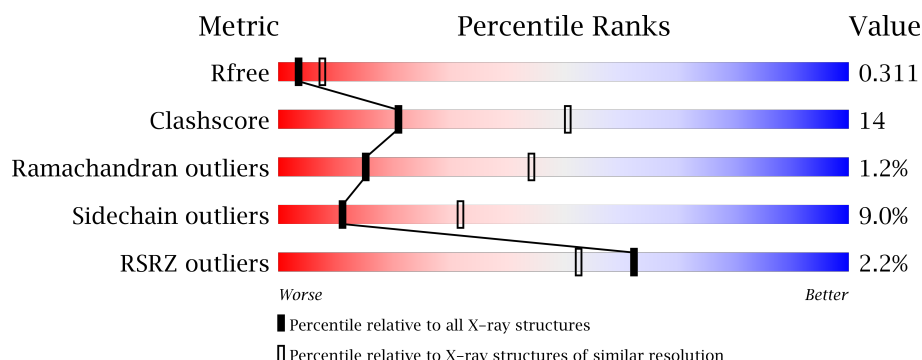
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div> <div></div> <div>61%</div> <div>34%</div> <div>5%</div> </div> <div> <div>0.1%</div> </div> </div>
1	B	289	<div> <div> <div></div> <div>61%</div> <div>32%</div> <div>6%</div> </div> <div> <div>4%</div> </div> </div>

## 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.

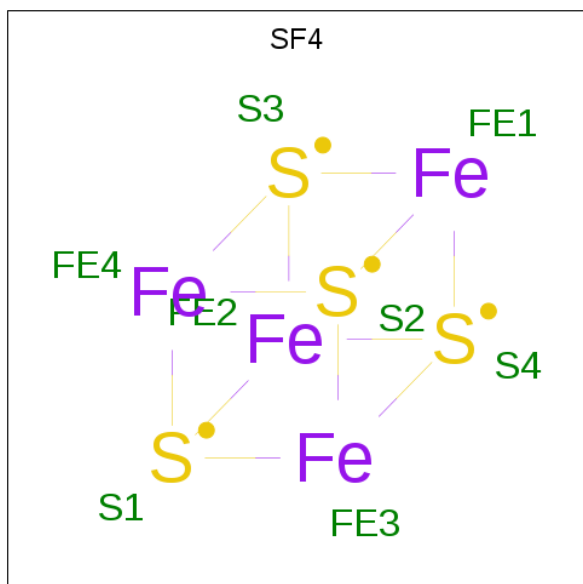
- Molecule 1 is a protein called Nitrogenase iron protein 1.

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	UNP P00459
B	129	GLU	ASP	ENGINEERED	UNP P00459

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

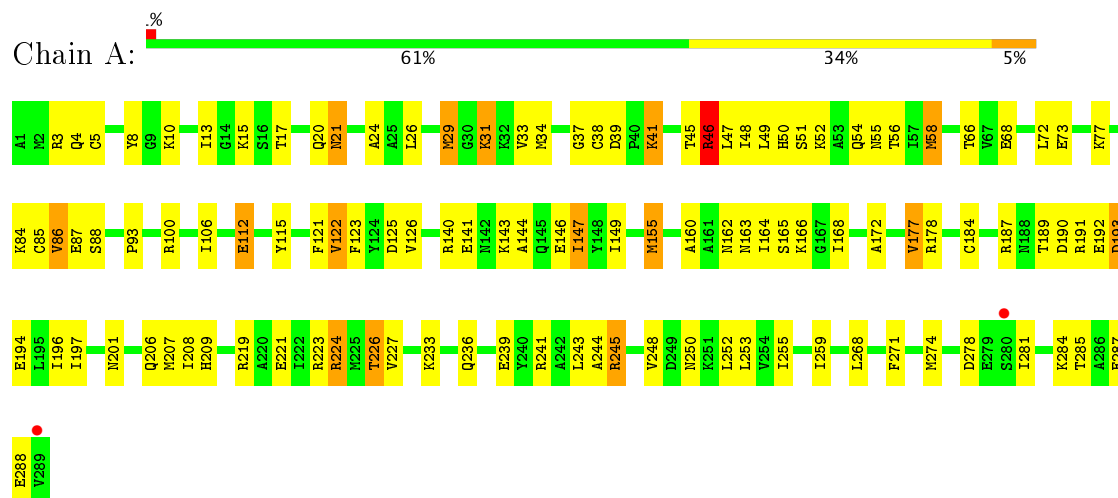


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		

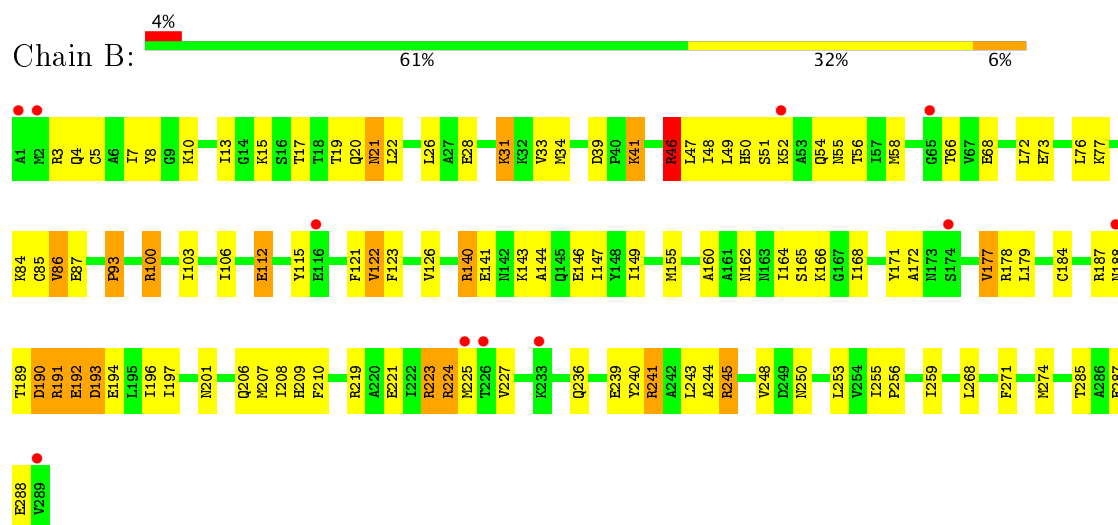
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, $\alpha$ , $\beta$ , $\gamma$	57.57Å 92.14Å 63.93Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.4 (20.00-2.80) 87.7 (19.78-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.79Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.227 , 0.299 0.241 , 0.311	Depositor DCC
$R_{free}$ test set	683 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.77	0/2212	1.73	25/2978 (0.8%)
1	B	0.80	0/2212	1.70	26/2978 (0.9%)
All	All	0.79	0/4424	1.72	51/5956 (0.9%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	ARG	NE-CZ-NH1	25.85	133.22	120.30
1	B	100	ARG	NE-CZ-NH2	22.80	131.70	120.30
1	A	100	ARG	NE-CZ-NH1	22.51	131.56	120.30
1	B	245	ARG	NE-CZ-NH2	20.79	130.69	120.30
1	B	100	ARG	NE-CZ-NH1	-20.60	110.00	120.30
1	A	100	ARG	NE-CZ-NH2	-20.12	110.24	120.30
1	A	245	ARG	NE-CZ-NH2	-18.89	110.86	120.30
1	B	245	ARG	NE-CZ-NH1	-15.91	112.35	120.30
1	B	100	ARG	CD-NE-CZ	14.61	144.05	123.60
1	A	245	ARG	CD-NE-CZ	14.60	144.04	123.60
1	B	245	ARG	CD-NE-CZ	14.49	143.89	123.60
1	A	100	ARG	CD-NE-CZ	14.10	143.34	123.60
1	B	241	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	A	241	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	B	46	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	241	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	B	241	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	219	ARG	NE-CZ-NH1	8.99	124.79	120.30
1	B	219	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	B	178	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	178	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	A	178	ARG	NE-CZ-NH2	-7.30	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	140	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	46	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	46	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	223	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	224	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	223	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	187	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	140	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	250	ASN	CA-C-N	-5.92	104.17	117.20
1	A	58	MET	CA-CB-CG	-5.92	103.24	113.30
1	B	191	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	A	86	VAL	CB-CA-C	-5.87	100.24	111.40
1	A	221	GLU	CA-CB-CG	5.77	126.10	113.40
1	A	187	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	221	GLU	CA-CB-CG	5.72	125.98	113.40
1	B	140	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	178	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	223	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	147	ILE	CG1-CB-CG2	-5.68	98.89	111.40
1	B	187	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	29	MET	CA-CB-CG	5.33	122.37	113.30
1	B	250	ASN	CA-C-N	-5.29	105.56	117.20
1	B	210	PHE	CA-C-N	-5.27	105.60	117.20
1	A	191	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	76	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	224	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	188	ASN	CA-C-N	-5.05	106.09	117.20
1	B	86	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

There are no planarity outliers.

## 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	2188	0	2199	59	0
1	B	2188	0	2200	64	0
2	A	8	0	0	0	0
All	All	4384	0	4399	120	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 14.

All (120) 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: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
1:B:21:ASN:HD21	1:B:227:VAL:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:ASP:O	1:A:197:ILE:HG13	2.11	0.50
1:A:20:GLN:HE21	1:A:48:ILE:HG12	1.76	0.50
1:B:196:ILE:HG22	1:B:207:MET:HG3	1.93	0.50
1:B:50:HIS:HA	1:B:224:ARG:O	2.11	0.50
1:B:49:LEU:HD11	1:B:77:LYS:HB3	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: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: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:285:THR:HG22	1:B:288:GLU:OE1	2.15	0.46
1:B:72:LEU:HB2	1:B:112:GLU:HG2	1.97	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
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:146:GLU:HG2	1:B:253:LEU:CD1	2.46	0.45
1:B:56:THR:HG22	1:B:87:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:MET:SD	1:A:155:MET:C	2.95	0.44
1:A:194:GLU:HG3	1:A:271:PHE:CE2	2.52	0.44
1:A:233:LYS:HB2	1:A:233:LYS:HE3	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:B:34:MET:HA	1:B:84:LYS:O	2.18	0.44
1:B:8:TYR:O	1:B:149:ILE:HA	2.17	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: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: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
1:A:31:LYS:HD2	1:A:31:LYS:N	2.34	0.41
1:B:149:ILE:HG23	1:B:164:ILE:HD12	2.03	0.41
1:B:10:LYS:O	1:B:13:ILE:HG12	2.21	0.41
1:B:7:ILE:HG21	1:B:19:THR:OG1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	287/289 (99%)	263 (92%)	21 (7%)	3 (1%)	18	50
1	B	287/289 (99%)	262 (91%)	21 (7%)	4 (1%)	13	39
All	All	574/578 (99%)	525 (92%)	42 (7%)	7 (1%)	15	44

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	ILE
1	B	46	ARG
1	A	46	ARG
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%)	211 (91%)	22 (9%)	10	29
1	B	233 / 233 (100%)	213 (91%)	20 (9%)	12	34
All	All	466 / 466 (100%)	424 (91%)	42 (9%)	11	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	31	LYS
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
1	A	206	GLN
1	A	226	THR
1	A	245	ARG
1	B	21	ASN
1	B	31	LYS
1	B	39	ASP
1	B	41	LYS
1	B	46	ARG

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Mol	Chain	Res	Type
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	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	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	163	ASN
1	A	206	GLN
1	B	4	GLN
1	B	20	GLN
1	B	21	ASN
1	B	107	ASN
1	B	162	ASN
1	B	163	ASN
1	B	206	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	290	1	-	0/0/48/48	4/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	290	SF4	FE2-FE4-S1-S3
2	A	290	SF4	FE1-FE3-S2-S4
2	A	290	SF4	FE3-FE4-S1-S2
2	A	290	SF4	FE1-FE2-S3-S4

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	289/289 (100%)	-0.17	2 (0%) 87 83	33, 74, 98, 100	0
1	B	289/289 (100%)	-0.04	11 (3%) 41 30	39, 80, 99, 100	0
All	All	578/578 (100%)	-0.11	13 (2%) 62 52	33, 77, 99, 100	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	4.0
1	B	65	GLY	3.5
1	B	188	ASN	3.4
1	B	233	LYS	2.7
1	B	225	MET	2.5
1	A	289	VAL	2.4
1	B	116	GLU	2.4
1	B	174	SER	2.3
1	B	289	VAL	2.2
1	A	280	SER	2.2
1	B	52	LYS	2.2
1	B	226	THR	2.2
1	B	2	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SF4	A	290	8/8	0.99	0.07	-2.68	19,27,32,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.