



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:21 AM UTC

PDB ID : 1FRV / pdb_00001frv
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDRO-
GENASE
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on : 1996-03-28
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.49

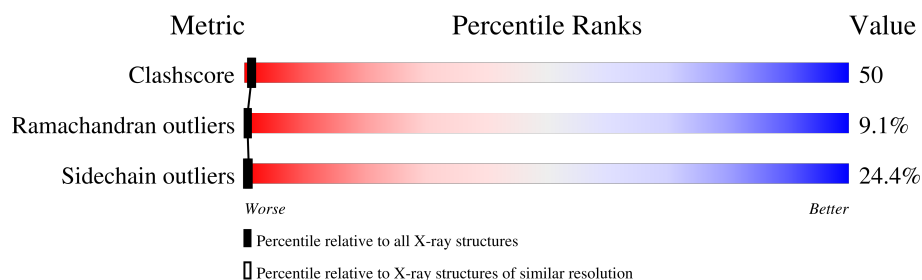
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

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	264	
1	C	264	
2	B	536	
2	D	536	

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
3	SF4	C	265	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12268 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.

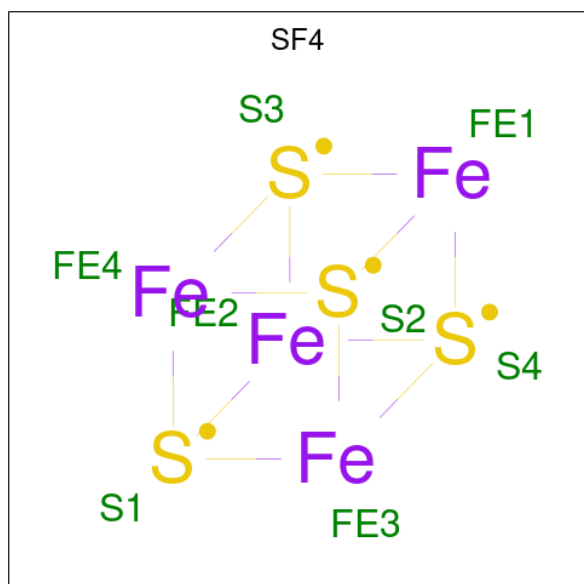
- Molecule 1 is a protein called HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			
1	C	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			

- Molecule 2 is a protein called HYDROGENASE.

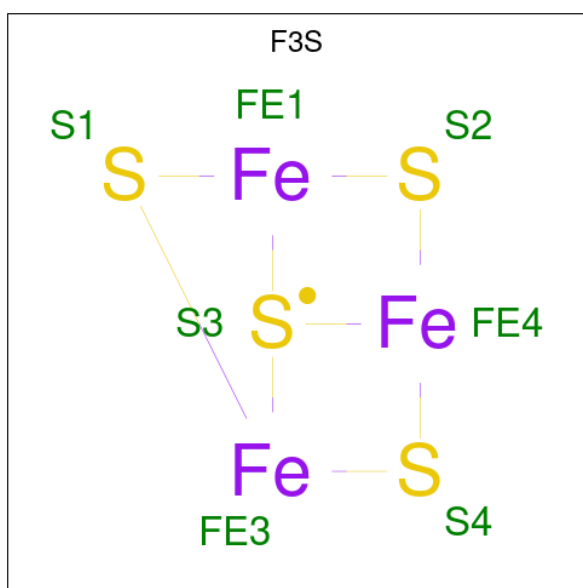
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			
2	D	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

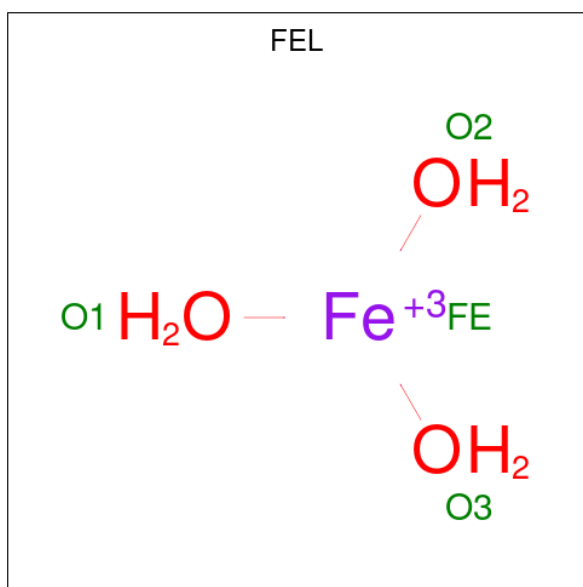


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		

- Molecule 6 is HYDRATED FE (CCD ID: FEL) (formula: FeH_6O_3).



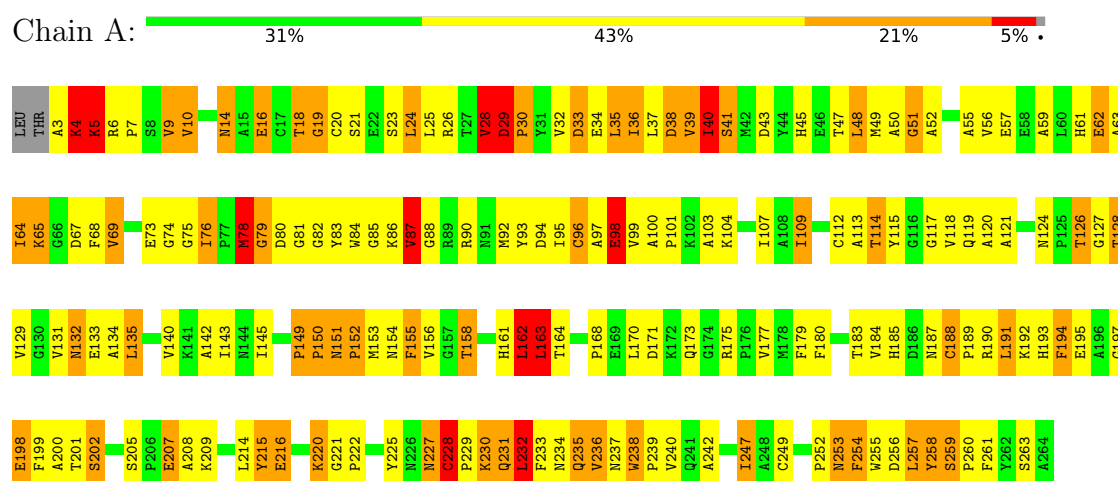
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	O	0	0
			4	1	3		
6	D	1	Total	Fe	O	0	0
			4	1	3		

3 Residue-property plots

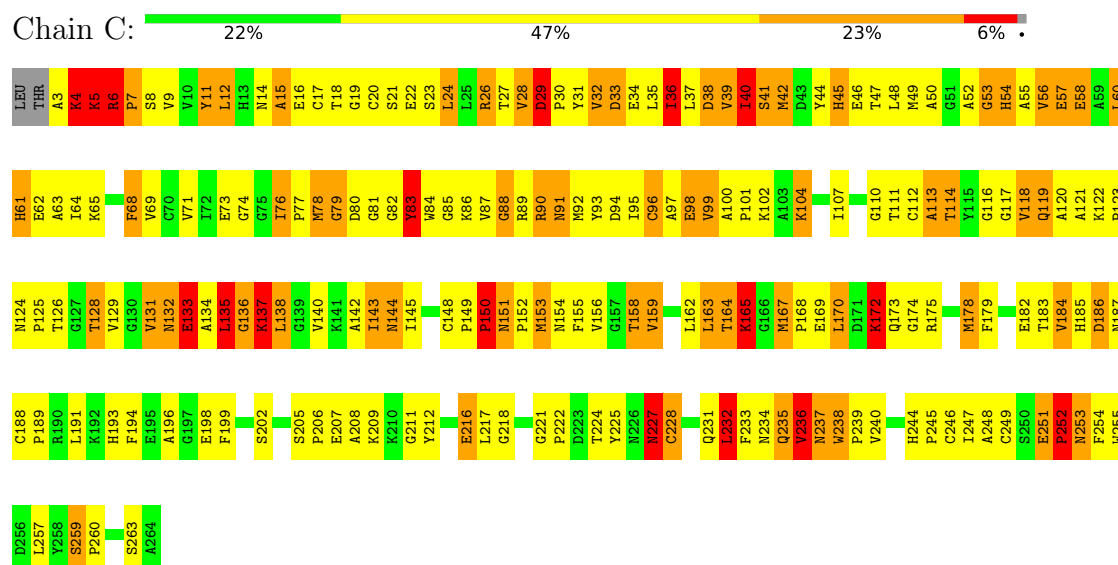
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

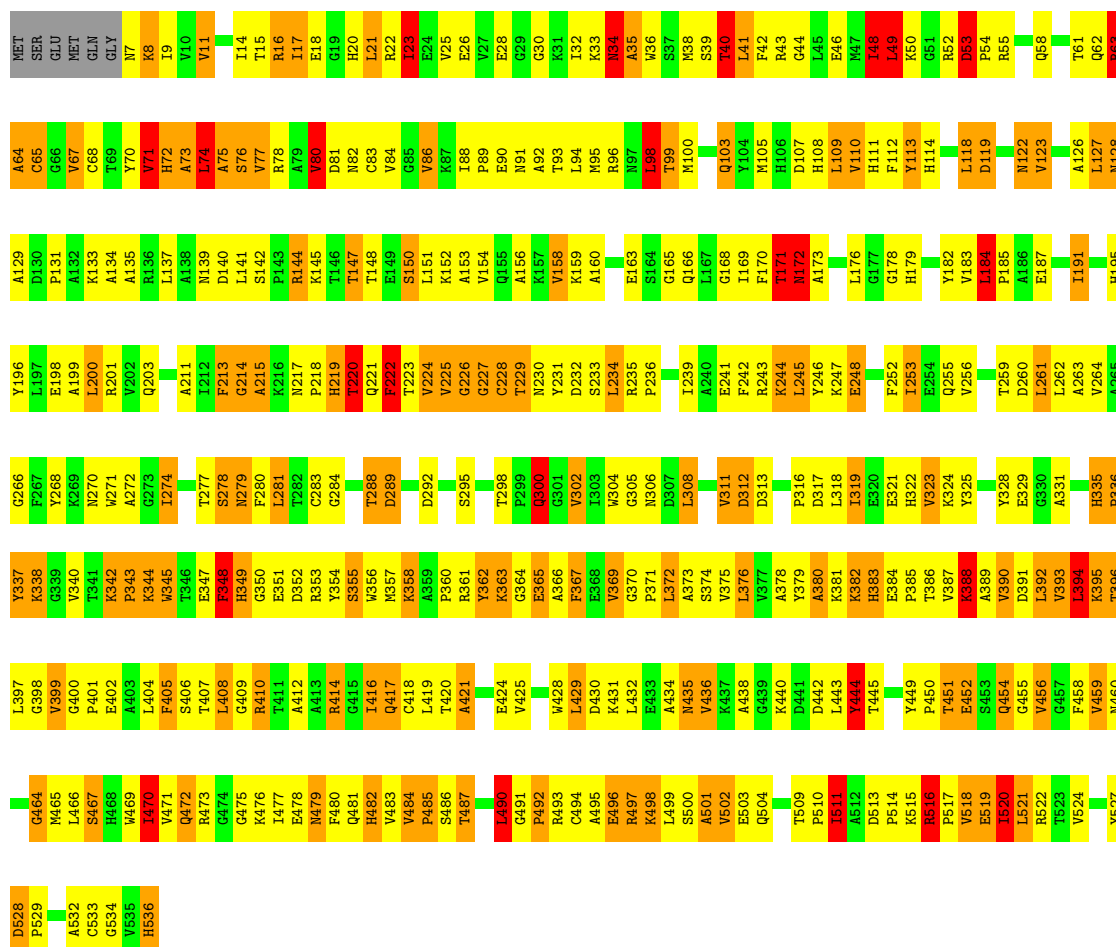


• Molecule 1: HYDROGENASE



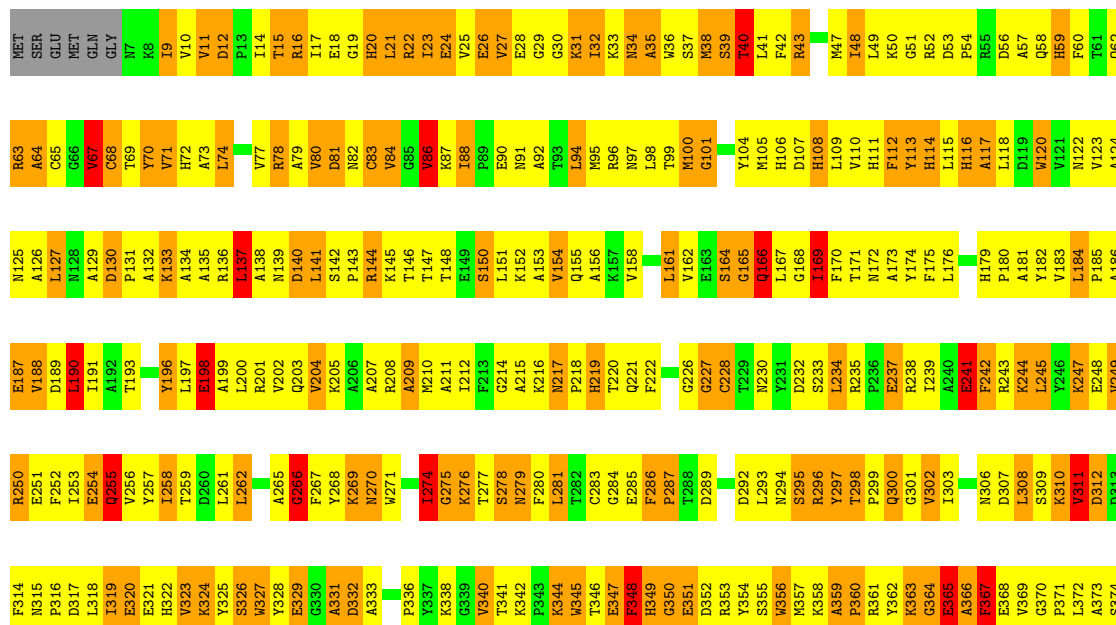
• Molecule 2: HYDROGENASE





● Molecule 2: HYDROGENASE

Chain D: 15% 48% 31% 5% ●



R497	R498	L499	S500	A501	S502	E503	S504	A505	L506	E507	S508	P509	P510	E511	A512	D513	P514	K515	R516	P517	S518	E519	I520	L521	R522	T523	V524	H525	S526	V527	D528	P529	C530	I531	A532	C533	G534	V535	H536																					
V436	A437	A438		D441	D442	L443	Y444	T445	D446	Y447	Q448	Y449	P450	T451	E452	S453	Q454	G455	V456	G457	F458	V459	M460	A461	P462	R463	G464	V465	L466	S467	H468	V469	L470	V471	Q472	R473	G474	G475	L476	L477	S478	N479	F480	Q481	H482	V483	V484	P485	S486	T487	H488	N489	L490	G491	P492	R493	C494	A495	F496	N497
V375	L376	V377	A378	V379	A380	K381	K382	H383	E384	P385	T386	V387	K388	A389	V390	D391	L392	V393	L394	K395	T396	L397	G398	V399	G400	P401	E402	A403	L404	F405	S406	T407	L408	G409	R410	T411	A412	A413	R414	G415	T416	Q417	C418	L419	T420	A421			E424	V425	E426	V427	N428	L429	D430	K431	L432	E433	A434	N435

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 93.90Å 69.20Å 89.80° 102.90° 90.80°	Depositor
Resolution (Å)	8.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.3 (8.00-2.85)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: NI, SF4, F3S, FEL

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	1.05	1/2014 (0.0%)	2.02	62/2738 (2.3%)
1	C	1.05	2/2014 (0.1%)	1.94	68/2738 (2.5%)
2	B	1.01	3/4251 (0.1%)	1.89	99/5782 (1.7%)
2	D	1.01	2/4251 (0.0%)	1.90	111/5782 (1.9%)
All	All	1.02	8/12530 (0.1%)	1.92	340/17040 (2.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	THR	CA-CB	7.32	1.60	1.53
2	D	491	GLY	N-CA	6.24	1.53	1.44
1	A	76	ILE	CA-CB	5.91	1.61	1.54
2	B	470	ILE	CA-CB	5.70	1.61	1.54
2	B	220	THR	CA-CB	5.41	1.61	1.53

The worst 5 of 340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	PHE	CA-CB-CG	14.91	128.71	113.80
1	A	76	ILE	N-CA-C	13.23	123.66	108.05
1	A	185	HIS	CA-CB-CG	12.21	126.00	113.80
2	D	366	ALA	N-CA-C	12.08	125.60	111.71
1	A	99	VAL	N-CA-C	11.35	121.83	110.82

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	1961	0	1879	162	0
1	C	1961	0	1879	207	0
2	B	4145	0	4073	382	1
2	D	4145	0	4073	513	1
3	A	16	0	0	2	0
3	C	16	0	0	3	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
All	All	12268	0	11904	1205	1

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 50.

The worst 5 of 1205 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:308:LEU:HD21	2:B:405:PHE:HZ	1.15	1.07
2:D:14:ILE:HG13	2:D:21:LEU:HD13	1.30	1.07
1:C:29:ASP:HB3	1:C:30:PRO:HD3	1.30	1.06
2:D:27:VAL:HG22	2:D:32:ILE:HA	1.38	1.02
1:A:29:ASP:HB3	1:A:30:PRO:HD3	1.41	1.01

All (1) 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)
2:B:430:ASP:OD2	2:D:31:LYS:NZ[1_565]	2.18	0.02

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	260/264 (98%)	198 (76%)	42 (16%)	20 (8%)	1	1
1	C	260/264 (98%)	192 (74%)	43 (16%)	25 (10%)	0	0
2	B	528/536 (98%)	387 (73%)	94 (18%)	47 (9%)	0	0
2	D	528/536 (98%)	379 (72%)	97 (18%)	52 (10%)	0	0
All	All	1576/1600 (98%)	1156 (73%)	276 (18%)	144 (9%)	0	0

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	29	ASP
1	A	41	SER
1	A	79	GLY
2	B	35	ALA

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	205/211 (97%)	158 (77%)	47 (23%)	1	0
1	C	205/211 (97%)	154 (75%)	51 (25%)	0	0
2	B	431/441 (98%)	335 (78%)	96 (22%)	1	0
2	D	431/441 (98%)	315 (73%)	116 (27%)	0	0
All	All	1272/1304 (98%)	962 (76%)	310 (24%)	1	0

5 of 310 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	184	LEU
2	D	446	ASP
2	D	217	ASN
2	D	311	VAL
2	D	502	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	HIS
2	D	34	ASN
2	D	504	GLN
1	C	124	ASN
1	C	235	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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	F3S	C	266	1	0,9,9	-	-	-		
6	FEL	D	537	2	0,3,3	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
6	FEL	B	537	2	0,3,3	-	-	-		

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
4	F3S	C	266	1	-	-	0/3/3/3
3	SF4	C	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	A	267	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	265	SF4	2	0
3	C	267	SF4	1	0
3	A	265	SF4	1	0
3	A	267	SF4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.