wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2024 – 04:15 PM EDT

PDB ID	:	1FRV
Title	:	CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
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 (i) 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 (i)) were used in the production of this report:

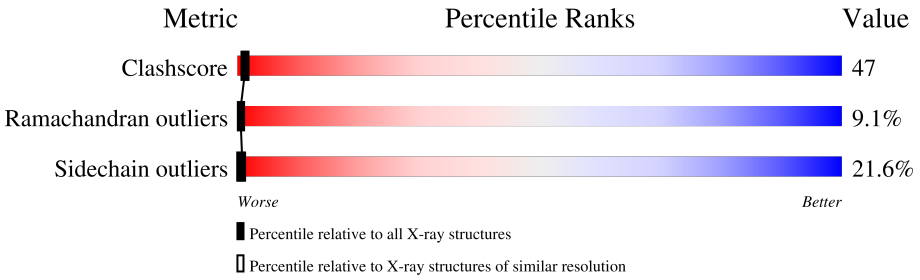
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	37% 44% 17%
1	C	264	29% 52% 16%
2	B	536	32% 47% 18%
2	D	536	18% 56% 22%

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.

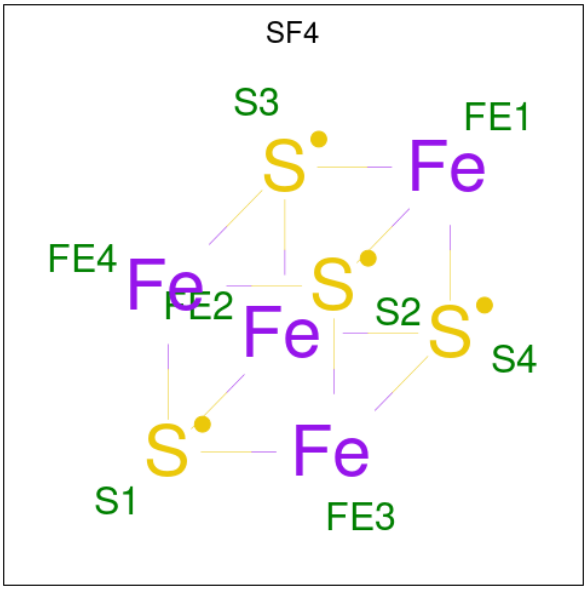
- Molecule 1 is a protein called HYDROGENASE.

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.

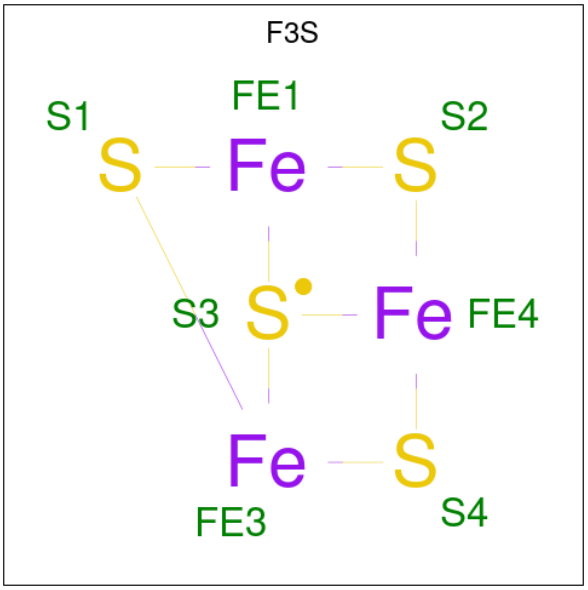
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			
2	D	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).

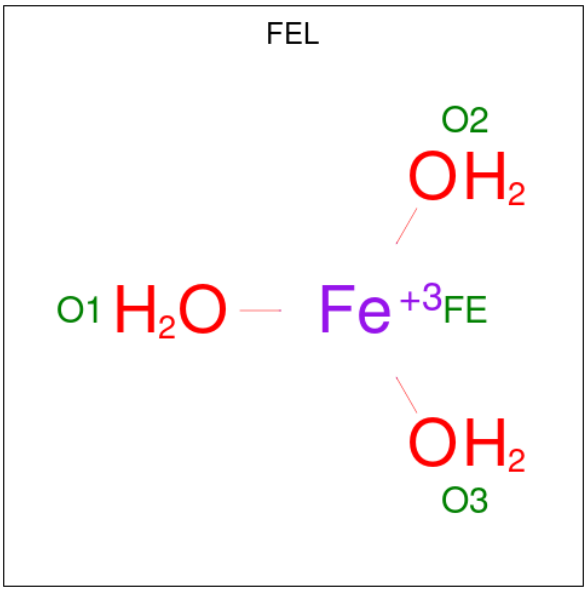


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 7 3 4	0	0
4	C	1	Total Fe S 7 3 4	0	0

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 6 is HYDRATED FE (three-letter code: FEL) (formula: FeH_6O_3).



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

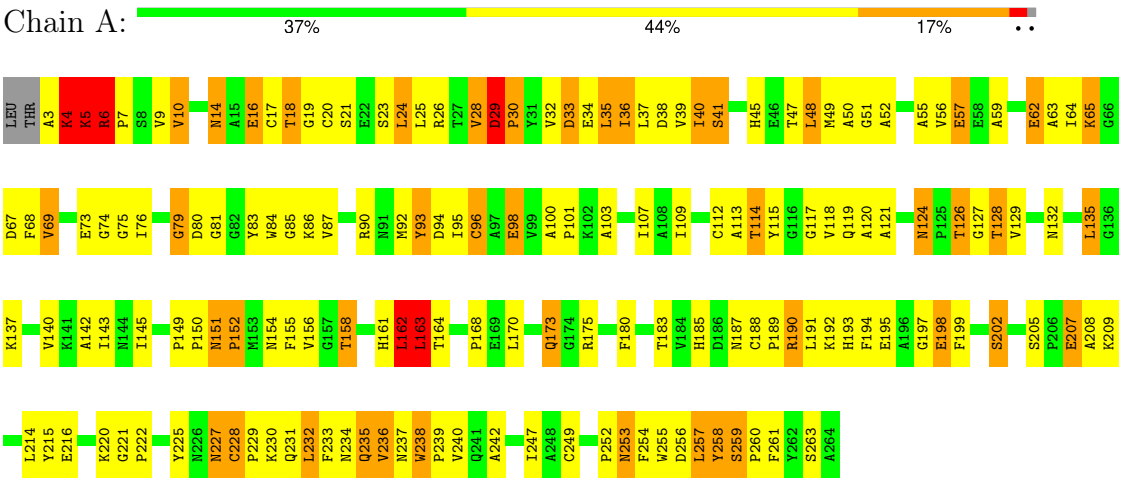
3 Residue-property plots (i)

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.

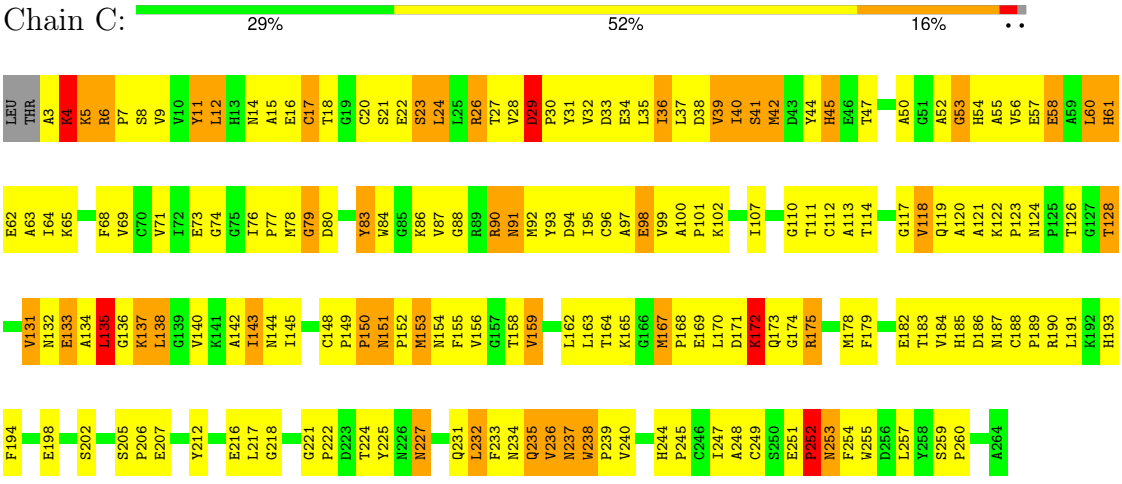
• Molecule 1: HYDROGENASE

Chain A:



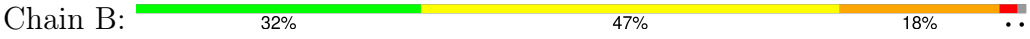
• Molecule 1: HYDROGENASE

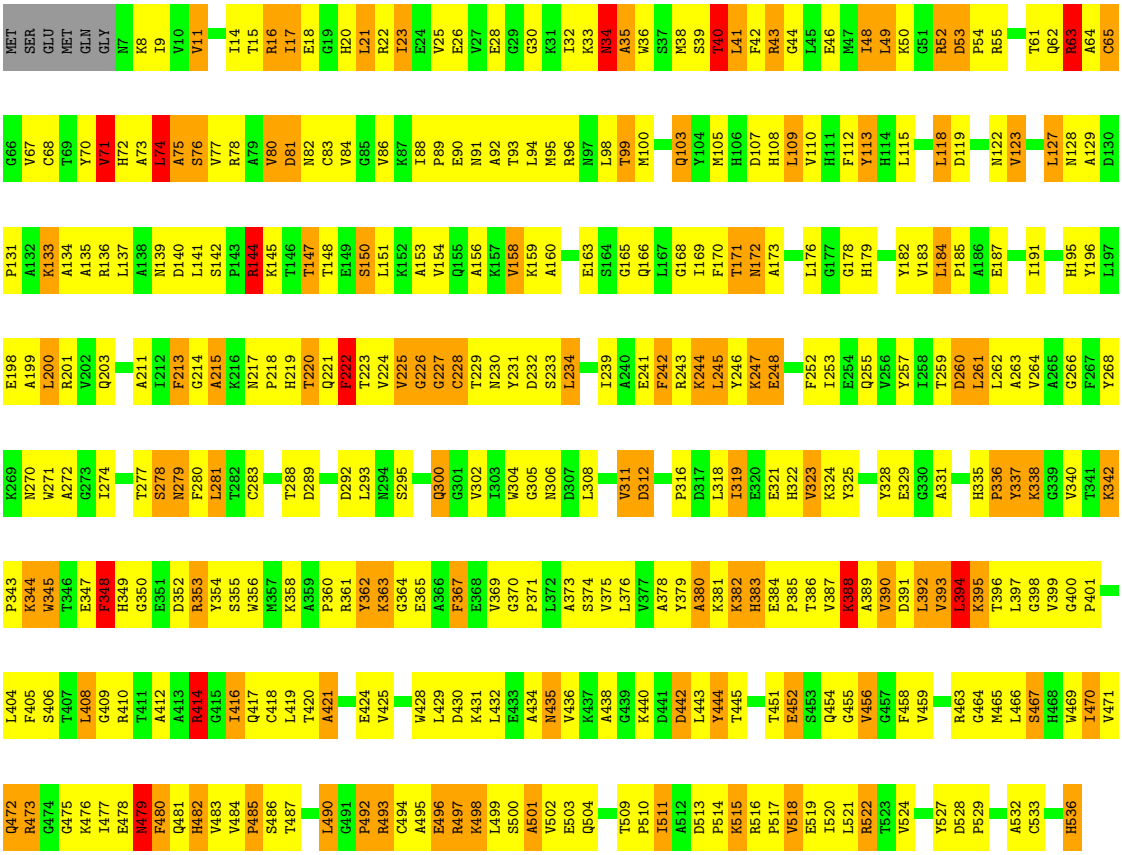
Chain C:



• Molecule 2: HYDROGENASE

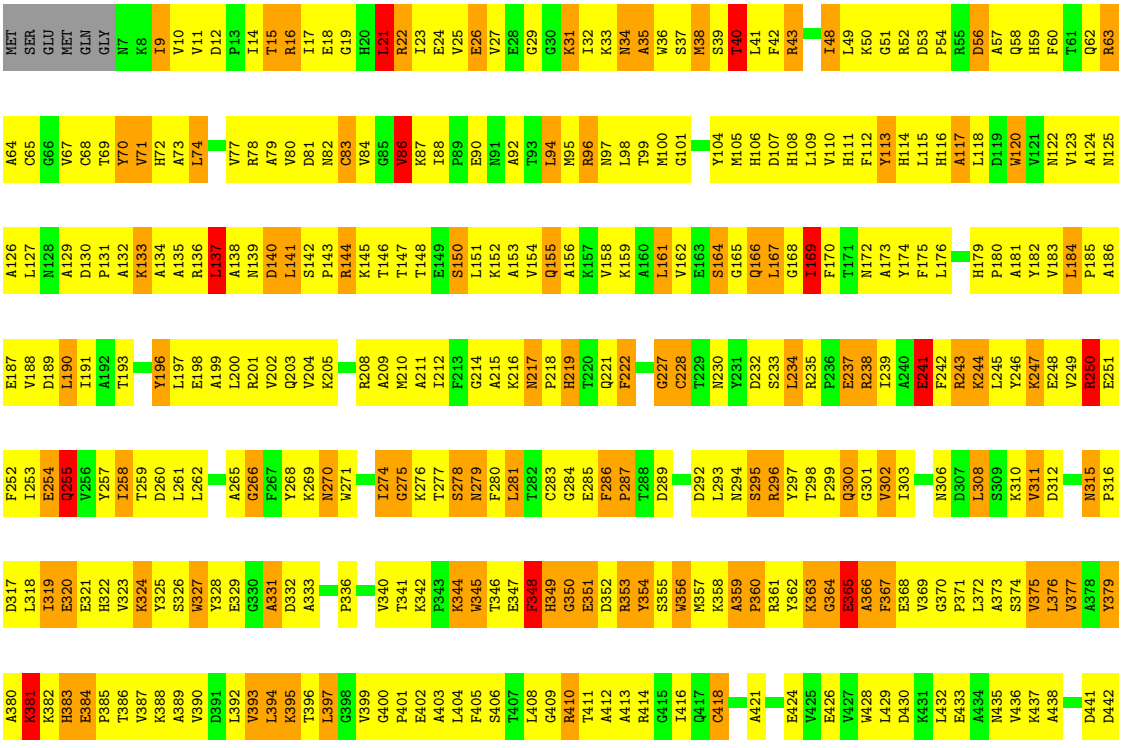
Chain B:

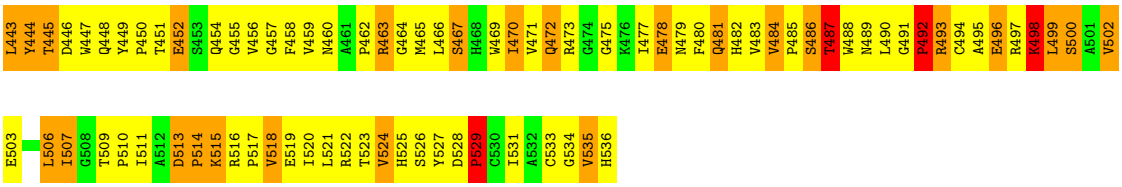




• Molecule 2: HYDROGENASE

Chain D:




L443
Y444
T445
D446
W447
Q448
Y449
P450
T451
E452
S453
Q454
G455
V456
G457
F458
V459
N460
A461
P462
R463
G464
M465
L466
S467
H468
W469
I470
V471
Q472
R473
G474
G475
K476
I477
E478
M479
F480
Q481
H482
V483
V484
P485
S486
T487
W488
N489
L490
G491
P492
R493
C494
A495
E496
R497
K498
L499
S500
A501
V502
E503
L506
I507
G508
T509
P510
I511
A512
D513
P514
K515
R516
P517
V518
E519
I520
L521
R522
T523
V524
H525
S526
Y527
D528
P529
C530
I531
A532
C533
G534
V535
H536

4 Data and refinement statistics (i)

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: SF4, F3S, NI, 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	0.84	0/2014	1.43	12/2738 (0.4%)
1	C	0.84	0/2014	1.44	11/2738 (0.4%)
2	B	0.81	0/4251	1.45	37/5782 (0.6%)
2	D	0.81	0/4251	1.45	36/5782 (0.6%)
All	All	0.82	0/12530	1.45	96/17040 (0.6%)

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	63	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	190	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	B	414	ARG	NE-CZ-NH1	11.16	125.88	120.30
2	D	16	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	74	GLY	N-CA-C	10.34	138.94	113.10

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	155	0
1	C	1961	0	1879	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4145	0	4073	362	1
2	D	4145	0	4073	487	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	1142	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 47.

The worst 5 of 1142 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 (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	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 (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	205/211 (97%)	160 (78%)	45 (22%)	1 0
1	C	205/211 (97%)	161 (78%)	44 (22%)	1 0
2	B	431/441 (98%)	346 (80%)	85 (20%)	1 1
2	D	431/441 (98%)	330 (77%)	101 (23%)	0 0
All	All	1272/1304 (98%)	997 (78%)	275 (22%)	1 0

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	326	SER
2	D	365	GLU
2	D	478	GLU
2	B	342	LYS
2	B	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	HIS
2	D	72	HIS
1	C	124	ASN
1	C	235	GLN
2	D	172	ASN

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	$\#\|Z\| > 2$
3	SF4	A	267	1	0,12,12	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
6	FEL	B	537	2	0,3,3	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
6	FEL	D	537	2	0,3,3	-	-	-		
3	SF4	C	265	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
3	SF4	A	267	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
3	SF4	C	265	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	A	267	SF4	1	0
3	A	265	SF4	1	0
3	C	267	SF4	1	0
3	C	265	SF4	2	0

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.