



wwPDB X-ray Structure Validation Summary Report

Sep 14, 2020 – 08:59 PM BST

PDB ID : 6Z7R
Title : Structure of [NiFeSe] hydrogenase from *Desulfovibrio vulgaris hildenborough* pressurized with Krypton gas - structure wtKr1
Authors : Zacarias, S.; Temporao, A.; Carpentier, P.; van der Linden, P.; Pereira, I.A.C.; Matias, P.M.
Deposited on : 2020-06-01
Resolution : 1.77 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

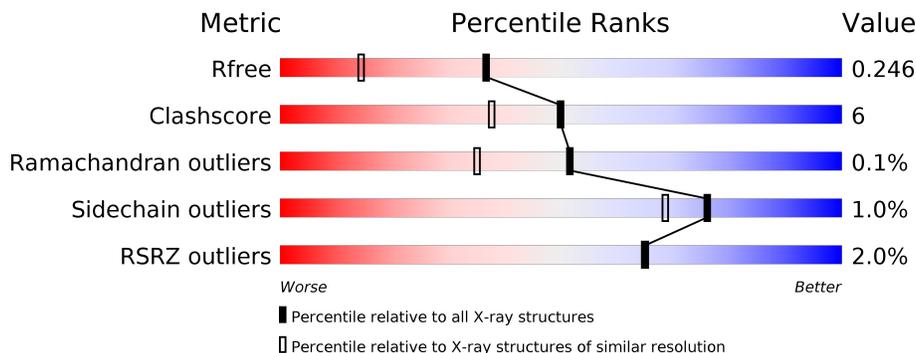
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 ≥ 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	283	 2% 85% 13% ..
1	C	283	 2% 87% 12% .
2	B	484	 2% 88% 12%
2	D	484	 2% 86% 13% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	KR	A	313	-	-	X	-
5	KR	B	507[B]	-	-	X	-
5	KR	B	508[B]	-	-	X	-
5	KR	B	510	-	-	X	-
5	KR	B	513	-	-	X	-
5	KR	C	314	-	-	X	-
5	KR	C	317	-	-	X	-
5	KR	D	506[B]	-	-	X	-
5	KR	D	508	-	-	X	-
5	KR	D	511	-	-	X	-
6	FCO	D	501	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 23815 atoms, of which 11678 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.

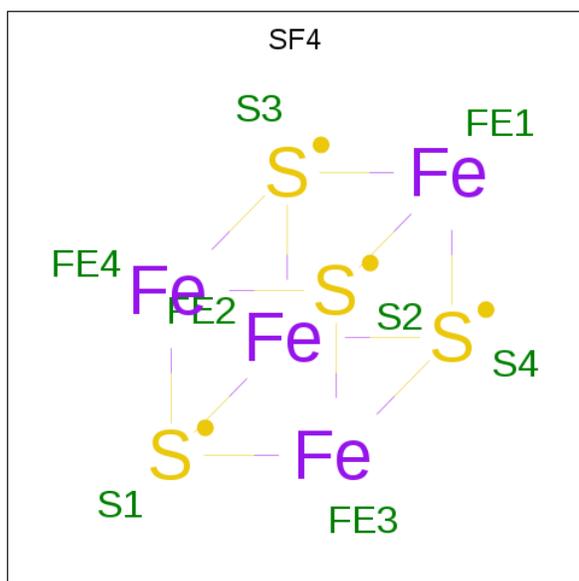
- Molecule 1 is a protein called Periplasmic [NiFeSe] hydrogenase, small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	279	4164	1346	2052	351	395	20	0	4	0
1	C	279	4163	1346	2051	351	395	20	0	4	0

- Molecule 2 is a protein called Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing.

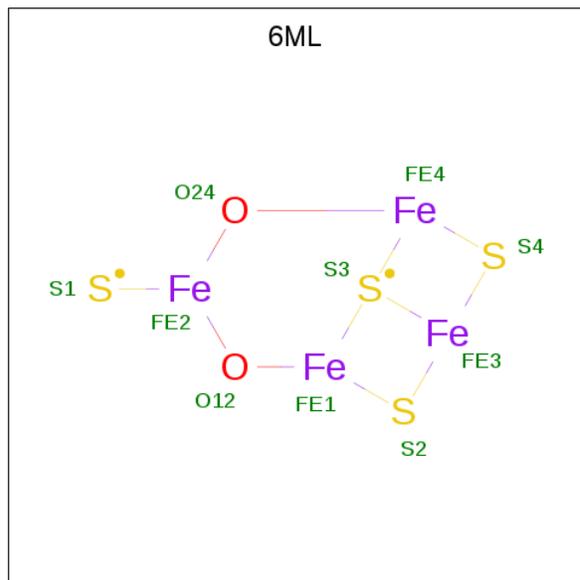
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
2	B	482	7556	2404	3788	655	687	19	3	0	6	0
2	D	481	7553	2403	3787	655	686	19	3	0	7	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: 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	A	1	Total	Fe	S	0	1
			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		
3	C	1	Total	Fe	S	0	1
			8	4	4		

- Molecule 4 is oxygen-damaged SF₄ (three-letter code: 6ML) (formula: Fe₄O₂S₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	O	S	0	1
			10	4	2	4		
4	C	1	Total	Fe	O	S	0	1
			10	4	2	4		

- Molecule 5 is KRYPTON (three-letter code: KR) (formula: Kr) (labeled as "Ligand of Interest" by author).

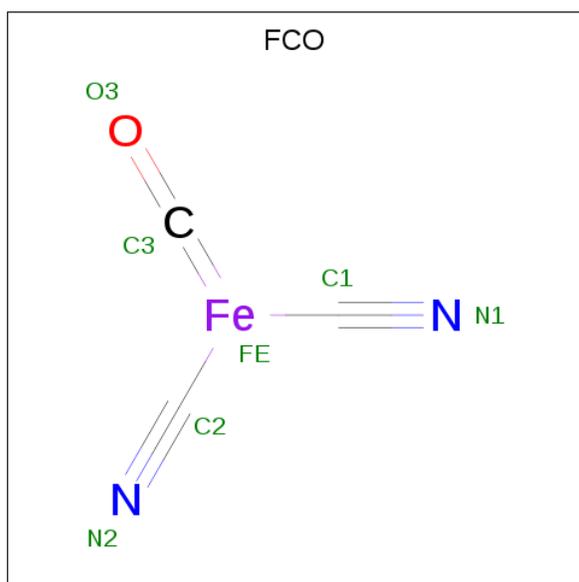
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	8	Total	Kr	0	4
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	Kr	0	2
			11	11		
5	D	7	Total	Kr	0	1
			8	8		
5	C	13	Total	Kr	0	3
			13	13		

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

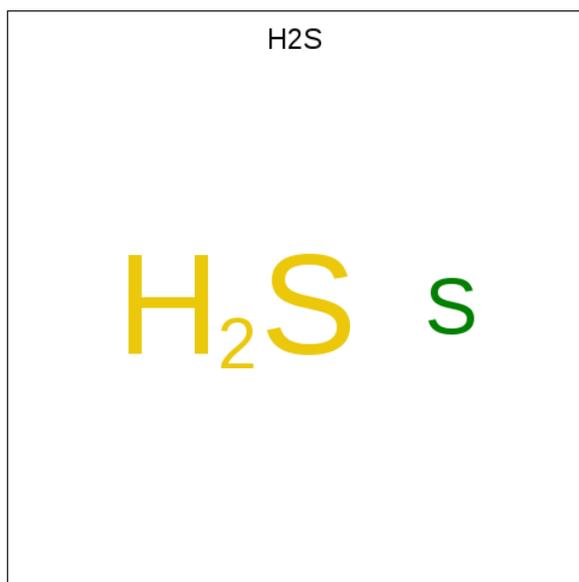
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe 1 1	0	0
8	D	1	Total Fe 1 1	0	0

- Molecule 9 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total S 1 1	0	0
9	D	1	Total S 1 1	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	D	1	Total Cl 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	42	Total O 42 42	0	0

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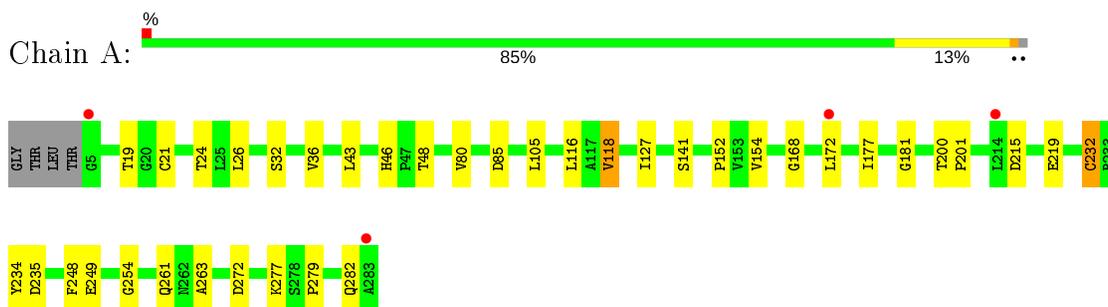
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	79	Total O 80 80	0	1
11	C	45	Total O 45 45	0	0
11	D	80	Total O 80 80	0	0

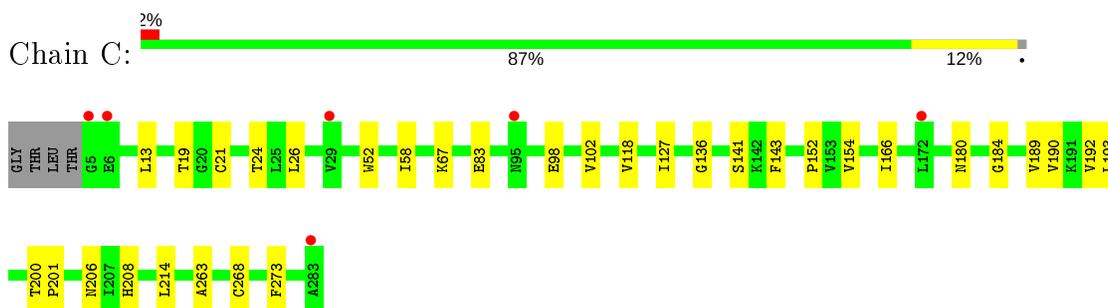
3 Residue-property plots [i](#)

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 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.

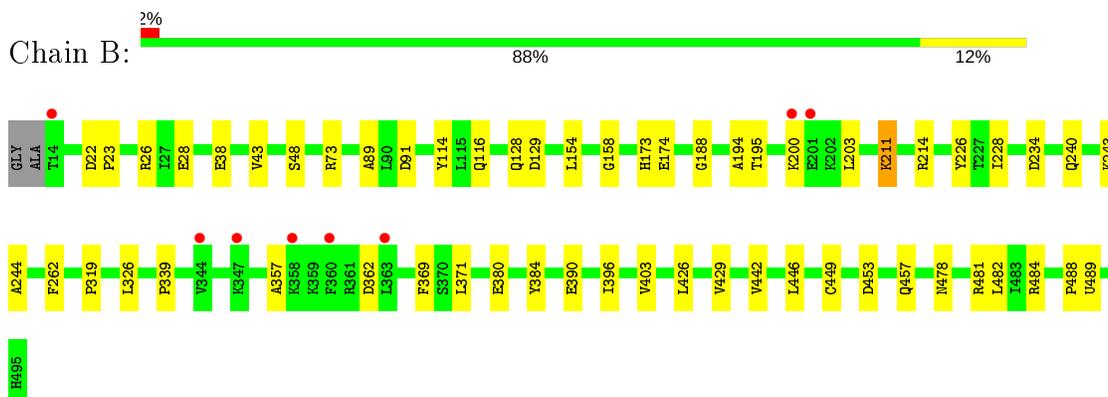
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit



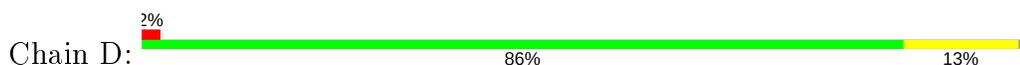
- Molecule 1: Periplasmic [NiFeSe] hydrogenase, small subunit

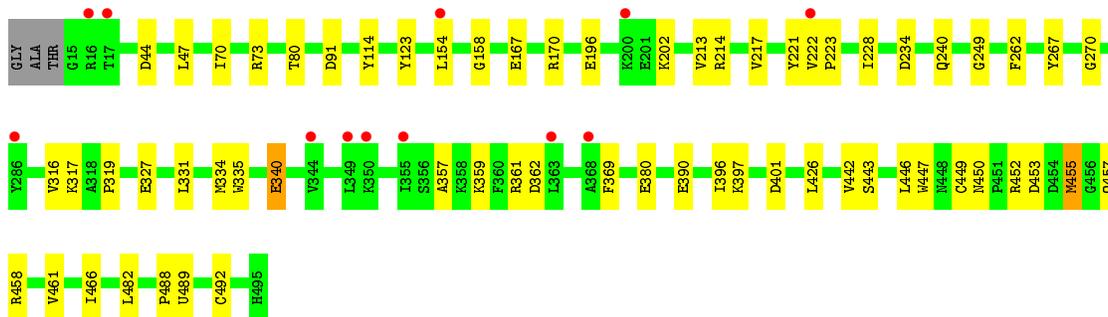


- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing



- Molecule 2: Periplasmic [NiFeSe] hydrogenase, large subunit, selenocysteine-containing





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.12Å 93.69Å 98.43Å 90.00° 93.26° 90.00°	Depositor
Resolution (Å)	58.05 – 1.77 67.81 – 1.77	Depositor EDS
% Data completeness (in resolution range)	75.7 (58.05-1.77) 75.7 (67.81-1.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.76Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.188 , 0.242 0.196 , 0.246	Depositor DCC
R_{free} test set	4804 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23815	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3760e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 6ML, CL, CSD, SF4, H2S, KR, SEC, FE2, FCO

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	0.64	0/2179	0.72	1/2960 (0.0%)
1	C	0.66	1/2179 (0.0%)	0.76	2/2960 (0.1%)
2	B	0.61	1/3853 (0.0%)	0.72	1/5209 (0.0%)
2	D	0.60	0/3854	0.76	2/5210 (0.0%)
All	All	0.62	2/12065 (0.0%)	0.74	6/16339 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	CYS	CB-SG	-6.45	1.71	1.82
2	B	262	PHE	C-N	-5.34	1.21	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	91	ASP	CB-CG-OD1	7.00	124.60	118.30
2	D	401	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	118	VAL	CG1-CB-CG2	-5.22	102.54	110.90
1	C	13	LEU	CB-CG-CD1	-5.08	102.36	111.00
2	B	91	ASP	CB-CG-OD1	5.05	122.85	118.30

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	2112	2052	2045	25	0
1	C	2112	2051	2045	21	0
2	B	3768	3788	3763	45	0
2	D	3766	3787	3762	46	0
3	A	24	0	0	0	0
3	C	24	0	0	0	0
4	A	10	0	0	2	0
4	C	10	0	0	1	0
5	A	11	0	0	5	0
5	B	10	0	0	12	0
5	C	13	0	0	10	0
5	D	8	0	0	10	0
6	B	7	0	0	1	0
6	D	7	0	0	2	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	1	0	0	1	0
9	D	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	A	42	0	0	2	0
11	B	80	0	0	3	0
11	C	45	0	0	2	0
11	D	80	0	0	0	0
All	All	12137	11678	11615	137	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 6.

The worst 5 of 137 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)
5:B:508[B]:KR:KR	5:B:509[B]:KR:KR	3.04	0.97
2:B:228:ILE:CD1	5:B:507[B]:KR:KR	2.89	0.82
2:B:384:TYR:CE2	5:B:513:KR:KR	2.99	0.76
1:C:98:GLU:OE2	11:C:401:HOH:O	2.10	0.70
2:B:384:TYR:CZ	5:B:513:KR:KR	3.08	0.68

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	281/283 (99%)	267 (95%)	13 (5%)	1 (0%)	34	19
1	C	281/283 (99%)	271 (96%)	9 (3%)	1 (0%)	34	19
2	B	483/484 (100%)	472 (98%)	11 (2%)	0	100	100
2	D	483/484 (100%)	470 (97%)	13 (3%)	0	100	100
All	All	1528/1534 (100%)	1480 (97%)	46 (3%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	263	ALA
1	A	263	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	227/226 (100%)	224 (99%)	3 (1%)	69	59
1	C	227/226 (100%)	224 (99%)	3 (1%)	69	59
2	B	396/391 (101%)	394 (100%)	2 (0%)	88	86
2	D	396/391 (101%)	392 (99%)	4 (1%)	76	68
All	All	1246/1234 (101%)	1234 (99%)	12 (1%)	76	68

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	TRP
1	C	67	LYS
2	D	114	TYR
2	B	211	LYS
2	D	80	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	260	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 2 are modelled with single atom and 48 are monoatomic - leaving 10 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	C	303[A]	1	0,12,12	0.00	-	-		
3	SF4	C	301	1	0,12,12	0.00	-	-		
4	6ML	A	304[B]	1	0,12,12	0.00	-	-		
6	FCO	D	501	2	0,6,6	0.00	-	-		
6	FCO	B	501	2	0,6,6	0.00	-	-		
4	6ML	C	304[B]	1	0,12,12	0.00	-	-		
3	SF4	A	303[A]	1	0,12,12	0.00	-	-		
3	SF4	A	301	1	0,12,12	0.00	-	-		
3	SF4	C	302	1	0,12,12	0.00	-	-		
3	SF4	A	302	1	0,12,12	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	C	303[A]	1	-	-	0/6/5/5
3	SF4	C	301	1	-	-	0/6/5/5
4	6ML	A	304[B]	1	-	-	0/2/3/3
4	6ML	C	304[B]	1	-	-	0/2/3/3
3	SF4	A	303[A]	1	-	-	0/6/5/5
3	SF4	A	301	1	-	-	0/6/5/5
3	SF4	C	302	1	-	-	0/6/5/5
3	SF4	A	302	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 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304[B]	6ML	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	FCO	2	0
6	B	501	FCO	1	0
4	C	304[B]	6ML	1	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 [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	279/283 (98%)	0.20	4 (1%) 75 75	14, 27, 47, 80	1 (0%)
1	C	279/283 (98%)	0.10	6 (2%) 62 61	12, 26, 46, 79	0
2	B	480/484 (99%)	0.06	8 (1%) 70 70	11, 27, 46, 62	1 (0%)
2	D	479/484 (98%)	0.16	12 (2%) 57 56	9, 29, 51, 74	2 (0%)
All	All	1517/1534 (98%)	0.13	30 (1%) 65 65	9, 27, 47, 80	4 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	5.0
2	D	154	LEU	4.2
2	D	349	LEU	3.6
2	B	201	GLU	3.3
2	D	344	VAL	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	CSD	D	75[A]	7/9	0.98	0.09	10,12,19,19	2
2	CSD	D	75[B]	7/9	0.98	0.09	10,13,19,19	1
2	CSD	B	75[B]	7/9	0.99	0.09	7,16,22,22	1
2	CSD	B	75[A]	7/9	0.99	0.09	7,16,22,22	2

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
5	KR	A	314	1/1	0.81	0.08	53,53,53,53	1
5	KR	D	507	1/1	0.91	0.08	49,49,49,49	0
5	KR	C	316	1/1	0.91	0.08	45,45,45,45	1
5	KR	D	510	1/1	0.92	0.10	46,46,46,46	1
5	KR	B	513	1/1	0.92	0.10	56,56,56,56	1
5	KR	C	311[B]	1/1	0.93	0.07	43,43,43,43	1
5	KR	D	508	1/1	0.95	0.08	41,41,41,41	1
5	KR	D	511	1/1	0.95	0.06	42,42,42,42	1
5	KR	C	314	1/1	0.96	0.06	57,57,57,57	1
5	KR	C	315	1/1	0.97	0.06	48,48,48,48	1
5	KR	B	512	1/1	0.97	0.06	49,49,49,49	1
5	KR	A	309[B]	1/1	0.97	0.06	51,51,51,51	1
5	KR	C	312[C]	1/1	0.97	0.08	24,24,24,24	1
5	KR	A	315	1/1	0.97	0.06	36,36,36,36	1
3	SF4	A	301	8/8	0.97	0.07	29,35,38,48	0
5	KR	D	512	1/1	0.97	0.04	48,48,48,48	1
5	KR	A	312	1/1	0.98	0.10	29,29,29,29	1
5	KR	A	313	1/1	0.98	0.09	50,50,50,50	1
5	KR	C	308	1/1	0.98	0.10	38,38,38,38	1
5	KR	B	510	1/1	0.98	0.08	42,42,42,42	1
5	KR	A	310	1/1	0.98	0.10	40,40,40,40	0
5	KR	A	308[A]	1/1	0.98	0.09	30,30,30,30	1
9	H2S	B	504	1/1	0.98	0.09	13,13,13,13	1
5	KR	C	317	1/1	0.98	0.19	12,12,12,12	1
5	KR	B	509[A]	1/1	0.98	0.07	36,36,36,36	1
5	KR	B	509[B]	1/1	0.98	0.07	43,43,43,43	1
5	KR	B	508[A]	1/1	0.99	0.07	21,21,21,21	1
6	FCO	D	501	7/7	0.99	0.10	14,17,20,27	0
3	SF4	A	302	8/8	0.99	0.09	19,23,26,27	0
5	KR	B	507[B]	1/1	0.99	0.10	14,14,14,14	1
5	KR	B	508[B]	1/1	0.99	0.07	46,46,46,46	1
5	KR	B	511	1/1	0.99	0.08	31,31,31,31	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	KR	C	309	1/1	0.99	0.11	31,31,31,31	1
5	KR	C	307	1/1	0.99	0.10	30,30,30,30	1
5	KR	C	305	1/1	0.99	0.08	49,49,49,49	0
5	KR	D	509	1/1	0.99	0.07	39,39,39,39	1
5	KR	D	506[B]	1/1	0.99	0.06	31,31,31,31	1
8	FE2	D	503	1/1	0.99	0.10	29,29,29,29	0
5	KR	A	305	1/1	0.99	0.10	34,34,34,34	1
3	SF4	C	301	8/8	0.99	0.07	22,25,32,33	0
3	SF4	A	303[A]	8/8	0.99	0.11	15,16,16,17	8
5	KR	D	506[A]	1/1	0.99	0.06	28,28,28,28	1
5	KR	C	313	1/1	0.99	0.11	42,42,42,42	0
5	KR	A	311	1/1	0.99	0.12	32,32,32,32	1
5	KR	C	310[A]	1/1	0.99	0.10	39,39,39,39	1
4	6ML	A	304[B]	10/10	0.99	0.12	15,16,19,22	10
5	KR	A	306	1/1	0.99	0.12	23,23,23,23	1
5	KR	C	306	1/1	0.99	0.11	28,28,28,28	1
7	NI	B	502	1/1	0.99	0.08	18,18,18,18	1
3	SF4	C	302	8/8	0.99	0.09	13,18,19,21	0
5	KR	B	506[A]	1/1	0.99	0.12	18,18,18,18	1
7	NI	D	502	1/1	0.99	0.07	21,21,21,21	0
8	FE2	B	503	1/1	1.00	0.09	21,21,21,21	0
10	CL	D	505	1/1	1.00	0.09	15,15,15,15	0
4	6ML	C	304[B]	10/10	1.00	0.11	11,15,19,20	10
5	KR	A	307	1/1	1.00	0.10	30,30,30,30	1
3	SF4	C	303[A]	8/8	1.00	0.11	13,15,17,17	8
10	CL	B	505	1/1	1.00	0.08	17,17,17,17	0
6	FCO	B	501	7/7	1.00	0.10	11,17,22,22	0
9	H2S	D	504	1/1	1.00	0.08	15,15,15,15	1

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.