Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:15 PM GMT

PDB ID	:	1SUF
Title	:	Carbon Monoxide Dehydrogenase from Carboxydothermus hydrogenoformans-Inactive state
Authors	:	Dobbek, H.; Svetlitchnyi, V.; Liss, J.; Meyer, O.
Deposited on	:	2004-03-26
Resolution	:	1.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

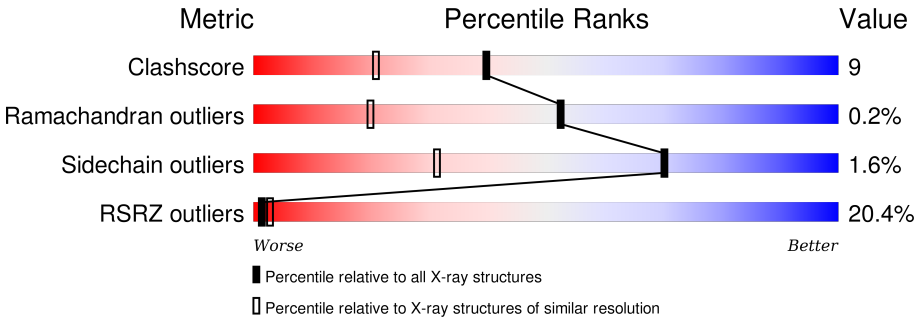
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.15 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	102246	1593 (1.20-1.08)
Ramachandran outliers	100387	1521 (1.20-1.08)
Sidechain outliers	100360	1518 (1.20-1.08)
RSRZ outliers	91569	1498 (1.20-1.08)

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. 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% 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	636	20% 85% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	A	638	-	-	-	X
4	NFS	A	639[A]	-	-	-	X
4	NFS	A	639[B]	-	-	-	X

2 Entry composition

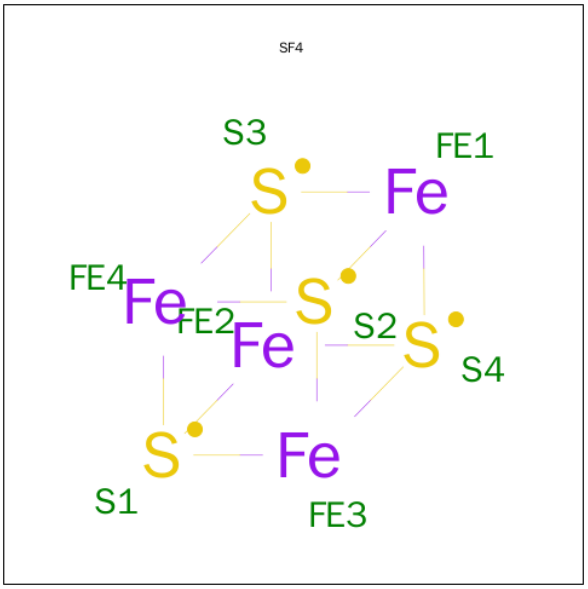
There are 5 unique types of molecules in this entry. The entry contains 5738 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carbon Monoxide Dehydrogenase 2.

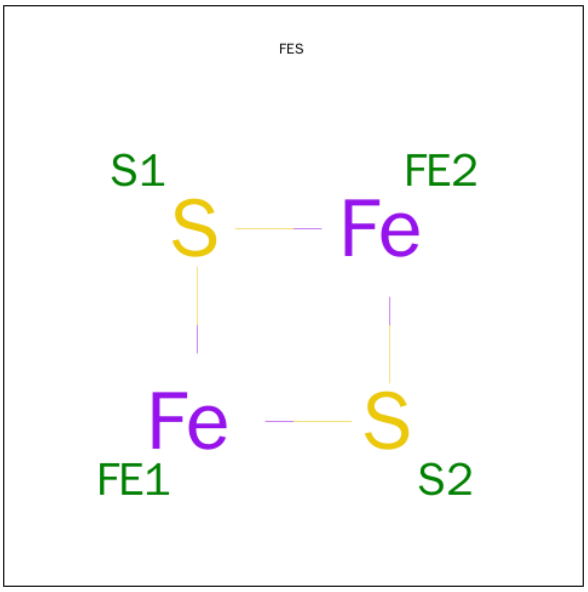
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	633	4653	2913	828	876	36	4	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



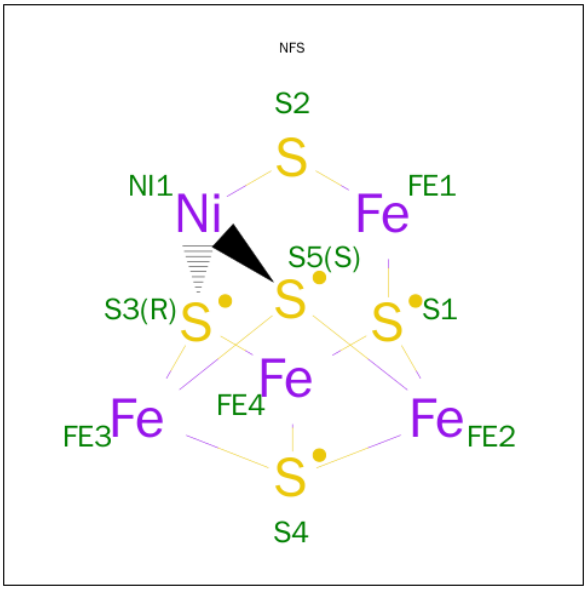
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 4 is FE(4)-NI(1)-S(5) CLUSTER (three-letter code: NFS) (formula: Fe_4NiS_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
4	A	1	10	5	1	4	0	1

- Molecule 5 is water.

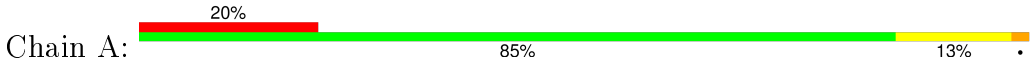
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1063	Total	O	0	0
			1063	1063		

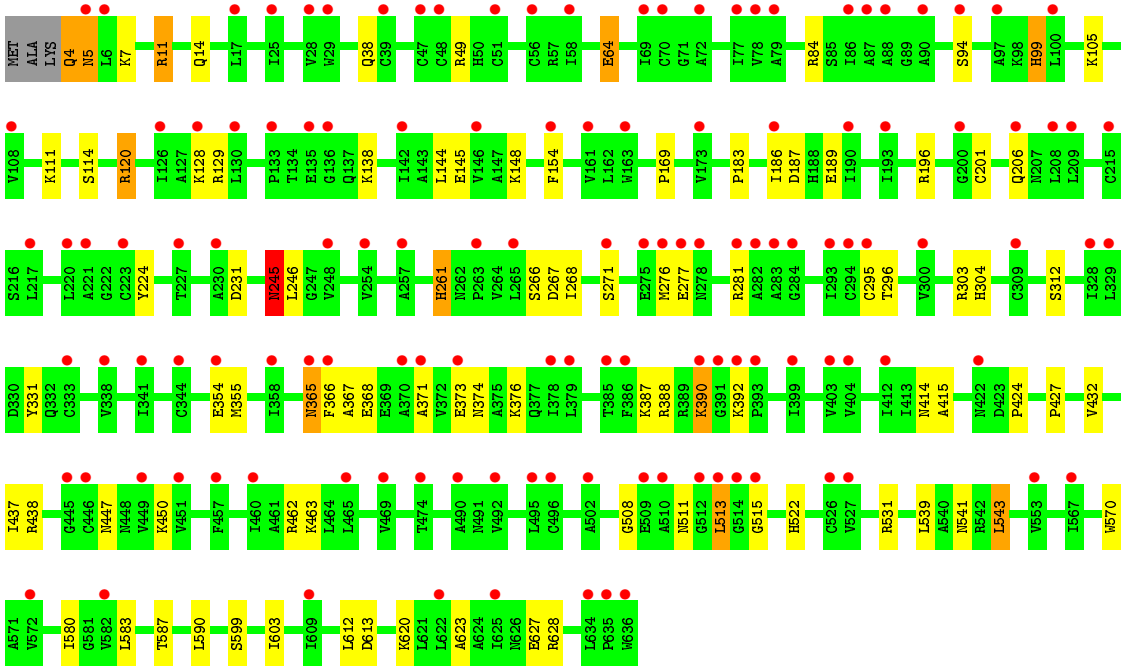
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Carbon Monoxide Dehydrogenase 2

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.61Å 75.00Å 71.37Å 90.00° 110.97° 90.00°	Depositor
Resolution (Å)	8.00 – 1.15 14.92 – 1.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.15) 91.7 (14.92-1.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.15Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.152 , 0.190 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 179646 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5738	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, NFS, FES

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	0.68	1/4725 (0.0%)	1.16	24/6418 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	SER	CB-OG	-5.48	1.35	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	120	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	A	570	TRP	CA-CB-CG	8.18	129.25	113.70
1	A	438	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	49	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	11	ARG	CD-NE-CZ	7.98	134.77	123.60
1	A	196	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	628	ARG	CD-NE-CZ	7.71	134.39	123.60
1	A	84	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	129	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	261	HIS	CA-CB-CG	-6.76	102.10	113.60
1	A	438	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	187	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	231	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	120	ARG	NH1-CZ-NH2	6.01	126.02	119.40
1	A	64	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	A	303	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	543	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	224	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	129	ARG	NE-CZ-NH2	-5.63	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	531	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	462	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	A	613	ASP	CB-CG-OD2	5.12	122.91	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	4653	0	4755	83	0
2	A	8	0	0	0	0
3	A	4	0	0	0	0
4	A	10	0	0	0	0
5	A	1063	0	0	50	0
All	All	5738	0	4755	83	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 9.

All (83) 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:A:128:LYS:HG2	5:A:1415:HOH:O	1.78	0.84
1:A:276:MET:HE1	1:A:376:LYS:HA	1.60	0.82
1:A:367:ALA:H	1:A:374:ASN:HD22	1.31	0.77
1:A:580:ILE:HB	5:A:1668:HOH:O	1.85	0.77
1:A:392:LYS:HE3	5:A:1489:HOH:O	1.87	0.74
1:A:94:SER:HB2	1:A:154:PHE:HE1	1.51	0.74
1:A:111:LYS:HE2	5:A:1689:HOH:O	1.88	0.72
1:A:373:GLU:HG2	5:A:1640:HOH:O	1.89	0.71
1:A:94:SER:HB3	5:A:1260:HOH:O	1.91	0.71
1:A:387:LYS:O	1:A:390:LYS:HG2	1.94	0.68
1:A:148:LYS:HG2	5:A:1247:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HG2	5:A:1651:HOH:O	1.94	0.67
1:A:138:LYS:HD3	5:A:1503:HOH:O	1.93	0.67
1:A:463:LYS:HD3	5:A:1016:HOH:O	1.94	0.67
1:A:271:SER:HB2	5:A:1653:HOH:O	1.95	0.66
1:A:94:SER:HB2	1:A:154:PHE:CE1	2.32	0.64
1:A:620:LYS:HE3	5:A:1645:HOH:O	1.98	0.63
1:A:354:GLU:HG2	5:A:1162:HOH:O	1.98	0.63
1:A:4:GLN:HA	1:A:4:GLN:HE21	1.65	0.62
1:A:11:ARG:HD3	5:A:1564:HOH:O	1.99	0.62
1:A:38:GLN:HE22	1:A:450:LYS:HE2	1.65	0.61
1:A:414:ASN:HB2	5:A:1647:HOH:O	1.98	0.61
1:A:612:LEU:HD23	5:A:1496:HOH:O	2.01	0.61
1:A:268:ILE:HA	5:A:1653:HOH:O	2.01	0.59
1:A:267:ASP:OD1	1:A:304:HIS:HE1	1.85	0.59
1:A:515:GLY:HA2	5:A:1538:HOH:O	2.01	0.59
1:A:388:ARG:HD2	5:A:1456:HOH:O	2.04	0.57
1:A:245:ASN:ND2	1:A:246:LEU:H	2.03	0.57
1:A:367:ALA:H	1:A:374:ASN:ND2	2.00	0.56
1:A:304:HIS:HD2	5:A:890:HOH:O	1.87	0.56
1:A:368:GLU:HG3	5:A:1439:HOH:O	2.06	0.55
1:A:268:ILE:HD12	5:A:1674:HOH:O	2.07	0.55
1:A:539:LEU:O	1:A:543:LEU:HD23	2.07	0.53
1:A:513:LEU:HD12	1:A:515:GLY:O	2.09	0.53
1:A:623:ALA:O	1:A:627:GLU:HG3	2.09	0.53
1:A:206:GLN:HE22	1:A:603:ILE:HD11	1.74	0.53
1:A:99:HIS:HD2	1:A:331:TYR:OH	1.92	0.53
1:A:148:LYS:HG3	5:A:1661:HOH:O	2.09	0.53
1:A:587:THR:HG22	5:A:820:HOH:O	2.09	0.53
1:A:114:SER:HA	5:A:1373:HOH:O	2.08	0.53
1:A:266:SER:HB3	1:A:296:THR:OG1	2.09	0.52
1:A:365:ASN:HD22	1:A:366:PHE:N	2.07	0.52
1:A:392:LYS:HG2	5:A:1515:HOH:O	2.08	0.52
1:A:4:GLN:HE22	1:A:7:LYS:NZ	2.08	0.52
1:A:169:PRO:HB2	5:A:822:HOH:O	2.10	0.51
1:A:111:LYS:HG2	5:A:1261:HOH:O	2.10	0.51
1:A:266:SER:HA	5:A:1648:HOH:O	2.09	0.51
1:A:105:LYS:HD2	5:A:1247:HOH:O	2.11	0.49
1:A:590:LEU:HD21	5:A:1678:HOH:O	2.11	0.49
1:A:245:ASN:HD22	1:A:246:LEU:H	1.59	0.49
1:A:276:MET:HE2	1:A:376:LYS:HG2	1.94	0.49
1:A:620:LYS:HG3	5:A:1645:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD21	1:A:148:LYS:HZ1	1.79	0.48
1:A:373:GLU:OE2	5:A:1556:HOH:O	2.20	0.47
1:A:4:GLN:N	5:A:1679:HOH:O	2.48	0.46
1:A:627:GLU:HG3	5:A:1237:HOH:O	2.15	0.46
1:A:4:GLN:N	5:A:1428:HOH:O	2.49	0.46
1:A:201:CYS:HB3	5:A:1694:HOH:O	2.16	0.46
1:A:144:LEU:HD12	5:A:1661:HOH:O	2.15	0.46
1:A:387:LYS:HE3	5:A:1565:HOH:O	2.16	0.46
1:A:105:LYS:HD2	5:A:1661:HOH:O	2.15	0.46
1:A:245:ASN:HD22	1:A:246:LEU:N	2.15	0.45
1:A:169:PRO:HB3	1:A:541:ASN:HD21	1.82	0.44
1:A:261:HIS:CD2	1:A:295:CYS:HB2	2.53	0.44
1:A:14:GLN:NE2	5:A:1482:HOH:O	2.49	0.44
1:A:371:ALA:HB3	5:A:1674:HOH:O	2.18	0.44
1:A:120:ARG:NE	5:A:1131:HOH:O	2.50	0.44
1:A:424:PRO:O	1:A:427:PRO:HD2	2.18	0.43
1:A:312:SER:HB3	1:A:447:ASN:HD22	1.83	0.43
1:A:583:LEU:HD11	1:A:587:THR:HG21	2.01	0.43
1:A:277:GLU:OE1	1:A:281:ARG:NH2	2.51	0.43
1:A:145:GLU:HG2	5:A:1057:HOH:O	2.19	0.43
1:A:415:ALA:HA	1:A:511:ASN:HD21	1.84	0.42
1:A:432:VAL:HA	1:A:437:ILE:O	2.20	0.42
1:A:392:LYS:NZ	5:A:1598:HOH:O	2.50	0.41
1:A:128:LYS:CG	5:A:1415:HOH:O	2.51	0.41
1:A:390:LYS:HA	5:A:1429:HOH:O	2.21	0.41
1:A:183:PRO:HB3	1:A:189:GLU:HG3	2.02	0.41
1:A:94:SER:CB	1:A:186:ILE:HG21	2.51	0.41
1:A:5:ASN:HB3	5:A:1482:HOH:O	2.20	0.41
1:A:508:GLY:O	1:A:513:LEU:HG	2.22	0.40
1:A:64:GLU:HG3	5:A:1196:HOH:O	2.21	0.40
1:A:114:SER:HB3	5:A:1674:HOH:O	2.22	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	631/636 (99%)	610 (97%)	20 (3%)	1 (0%)	52 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ASN

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	496/498 (100%)	488 (98%)	8 (2%)	70 31

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	ASN
1	A	99	HIS
1	A	245	ASN
1	A	365	ASN
1	A	390	LYS
1	A	513	LEU
1	A	522	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	GLN
1	A	38	GLN
1	A	59	ASN
1	A	99	HIS

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Mol	Chain	Res	Type
1	A	109	GLN
1	A	137	GLN
1	A	206	GLN
1	A	245	ASN
1	A	278	ASN
1	A	304	HIS
1	A	365	ASN
1	A	374	ASN
1	A	377	GLN
1	A	436	ASN
1	A	447	ASN
1	A	491	ASN
1	A	511	ASN
1	A	541	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are 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	637	1	0,12,12	0.00	-	0,24,24	0.00	-
3	FES	A	638	1,3	0,4,4	0.00	-	0,4,4	0.00	-
4	NFS	A	639[A]	1,5	0,12,14	0.00	-	0,22,26	0.00	-
4	NFS	A	639[B]	1	0,12,14	0.00	-	0,22,26	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	637	1	-	0/0/48/48	0/6/5/5
3	FES	A	638	1,3	-	0/0/4/4	0/1/1/1
4	NFS	A	639[A]	1,5	-	0/0/40/49	0/2/4/5
4	NFS	A	639[B]	1	-	0/0/40/49	0/2/4/5

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

6.1 Protein, DNA and RNA chains

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^{th} 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	633/636 (99%)	1.48	129 (20%) 1 3	8, 13, 30, 48	2 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	LEU	9.1
1	A	512	GLY	6.5
1	A	283	ALA	5.1
1	A	391	GLY	4.8
1	A	282	ALA	4.8
1	A	135	GLU	4.2
1	A	365	ASN	4.1
1	A	136	GLY	4.1
1	A	344	CYS	4.0
1	A	281	ARG	3.9
1	A	6	LEU	3.8
1	A	278	ASN	3.6
1	A	393	PRO	3.5
1	A	5	ASN	3.5
1	A	636	TRP	3.5
1	A	390	LYS	3.5
1	A	515	GLY	3.4
1	A	275	GLU	3.2
1	A	373	GLU	3.1
1	A	271	SER	3.0
1	A	379	LEU	2.9
1	A	190	ILE	2.9
1	A	341	ILE	2.8
1	A	56	CYS	2.8
1	A	108	VAL	2.8
1	A	69	ILE	2.8
1	A	161	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	186	ILE	2.7
1	A	276	MET	2.7
1	A	294	CYS	2.7
1	A	469	VAL	2.7
1	A	527	VAL	2.7
1	A	309	CYS	2.7
1	A	126	ILE	2.7
1	A	220	LEU	2.7
1	A	215	CYS	2.6
1	A	328	ILE	2.6
1	A	265	LEU	2.6
1	A	392	LYS	2.6
1	A	193	ILE	2.6
1	A	366	PHE	2.6
1	A	609	ILE	2.6
1	A	460	ILE	2.6
1	A	572	VAL	2.6
1	A	333	CYS	2.5
1	A	338	VAL	2.5
1	A	509	GLU	2.5
1	A	635	PRO	2.5
1	A	142	ILE	2.5
1	A	248	VAL	2.4
1	A	490	ALA	2.4
1	A	130	LEU	2.4
1	A	70	CYS	2.4
1	A	77	ILE	2.4
1	A	293	ILE	2.4
1	A	465	LEU	2.4
1	A	48	CYS	2.4
1	A	206	GLN	2.4
1	A	277	GLU	2.4
1	A	100	LEU	2.4
1	A	146	VAL	2.3
1	A	386	PHE	2.3
1	A	230	ALA	2.3
1	A	217	LEU	2.3
1	A	634	LEU	2.3
1	A	47	CYS	2.3
1	A	329	LEU	2.3
1	A	94	SER	2.3
1	A	227	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	88	ALA	2.3
1	A	223	CYS	2.3
1	A	208	LEU	2.2
1	A	553	VAL	2.2
1	A	582	VAL	2.2
1	A	25	ILE	2.2
1	A	86	ILE	2.2
1	A	72	ALA	2.2
1	A	257	ALA	2.2
1	A	370	ALA	2.2
1	A	514	GLY	2.2
1	A	209	LEU	2.2
1	A	133	PRO	2.2
1	A	358	ILE	2.2
1	A	625	ILE	2.2
1	A	510	ALA	2.2
1	A	154	PHE	2.2
1	A	378	ILE	2.2
1	A	200	GLY	2.2
1	A	51	CYS	2.2
1	A	446	CYS	2.2
1	A	526	CYS	2.2
1	A	17	LEU	2.1
1	A	90	ALA	2.1
1	A	502	ALA	2.1
1	A	354	GLU	2.1
1	A	58	ILE	2.1
1	A	385	THR	2.1
1	A	399	ILE	2.1
1	A	412	ILE	2.1
1	A	29	TRP	2.1
1	A	163	TRP	2.1
1	A	39	CYS	2.1
1	A	97	ALA	2.1
1	A	221	ALA	2.1
1	A	495	LEU	2.1
1	A	404	VAL	2.1
1	A	449	VAL	2.1
1	A	492	VAL	2.1
1	A	284	GLY	2.1
1	A	263	PRO	2.1
1	A	622	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	451	VAL	2.1
1	A	128	LYS	2.1
1	A	87	ALA	2.1
1	A	300	VAL	2.0
1	A	403	VAL	2.0
1	A	422	ASN	2.0
1	A	457	PHE	2.0
1	A	371	ALA	2.0
1	A	567	ILE	2.0
1	A	474	THR	2.0
1	A	445	GLY	2.0
1	A	295	CYS	2.0
1	A	496	CYS	2.0
1	A	28	VAL	2.0
1	A	78	VAL	2.0
1	A	173	VAL	2.0
1	A	254	VAL	2.0
1	A	79	ALA	2.0

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^{th} 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(Å^2)	Q<0.9
4	NFS	A	639[B]	9/10	0.96	0.19	4.71	0,1,11,13	2
4	NFS	A	639[A]	9/10	0.96	0.19	4.71	0,1,11,13	2
3	FES	A	638	4/4	0.96	0.16	3.75	0,0,8,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SF4	A	637	8/8	0.97	0.13	-0.17	0,0,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.