



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:23 PM GMT

PDB ID : 4ENU
Title : Structure of the S234D variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2012-04-13
Resolution : 1.70 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

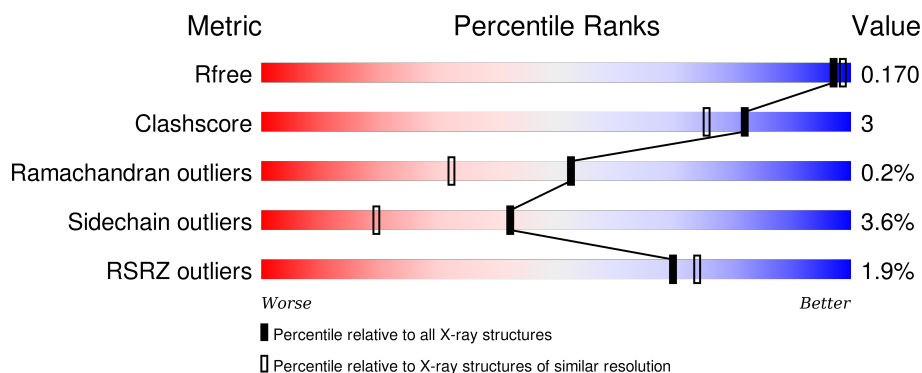
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 $\leq 5\%$. 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	753	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	753	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	753	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
1	D	753	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26286 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.

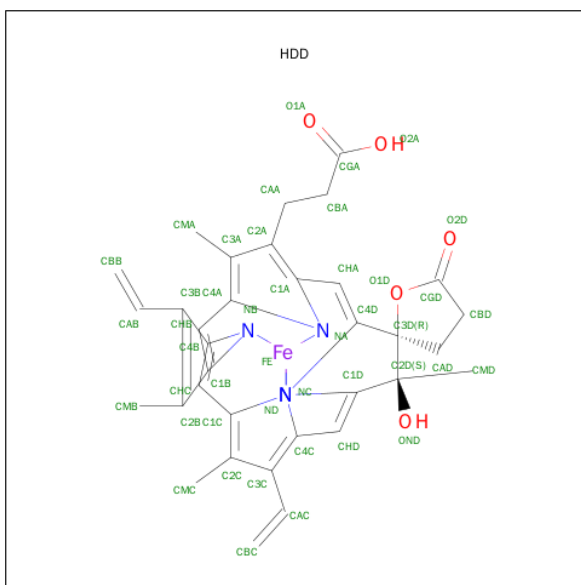
- Molecule 1 is a protein called Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5761	3656	1006	1087	12			
1	B	726	Total	C	N	O	S	0	3	0
			5758	3654	1006	1086	12			
1	C	726	Total	C	N	O	S	0	6	0
			5773	3665	1008	1088	12			
1	D	726	Total	C	N	O	S	0	4	0
			5765	3661	1006	1086	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
B	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
C	234	ASP	SER	ENGINEERED MUTATION	UNP P21179
D	234	ASP	SER	ENGINEERED MUTATION	UNP P21179

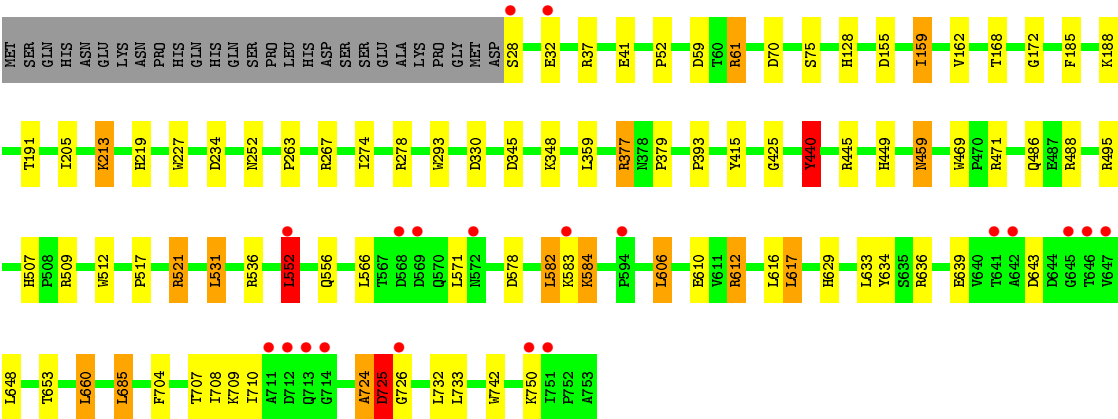
- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



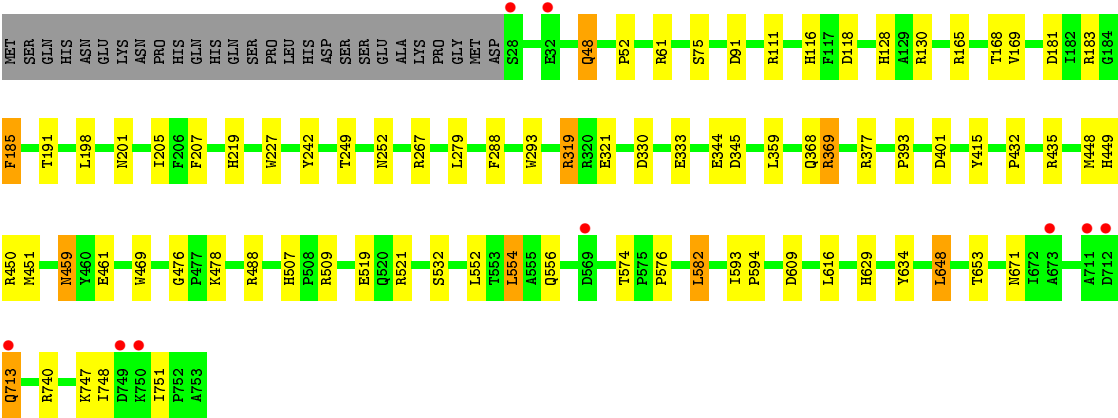
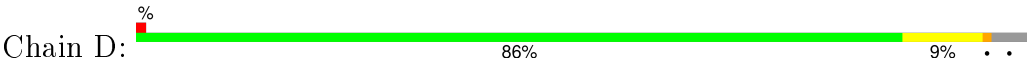
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	0
2	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	802	Total O 802 802	0	0
3	B	708	Total O 708 708	0	0
3	C	727	Total O 727 727	0	0
3	D	816	Total O 816 816	0	0



● Molecule 1: Catalase HP1I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.56Å 132.61Å 122.81Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	32.11 – 1.70 32.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (32.11-1.70) 91.7 (32.11-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.134 , 0.170 0.134 , 0.170	Depositor DCC
R_{free} test set	14327 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 283868 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26286	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: OCS, HDD

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	1.25	9/5920 (0.2%)	1.18	32/8047 (0.4%)
1	B	1.18	6/5914 (0.1%)	1.15	28/8039 (0.3%)
1	C	1.20	11/5937 (0.2%)	1.13	25/8069 (0.3%)
1	D	1.24	9/5925 (0.2%)	1.16	26/8054 (0.3%)
All	All	1.22	35/23696 (0.1%)	1.16	111/32209 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	TYR	CE1-CZ	9.84	1.51	1.38
1	D	333	GLU	CD-OE2	-7.73	1.17	1.25
1	C	469	TRP	CD2-CE2	7.67	1.50	1.41
1	A	321	GLU	CD-OE1	6.50	1.32	1.25
1	B	440	TYR	CE2-CZ	6.31	1.46	1.38

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	C	377	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	B	521	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	D	521	ARG	NE-CZ-NH2	-8.63	115.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	LEU	CB-CG-CD1	8.54	125.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5761	0	5593	28	1
1	B	5758	0	5589	41	1
1	C	5773	0	5612	41	0
1	D	5765	0	5598	37	0
2	A	44	0	31	2	0
2	B	44	0	31	1	0
2	C	44	0	31	4	0
2	D	44	0	31	3	0
3	A	802	0	0	9	1
3	B	708	0	0	8	0
3	C	727	0	0	9	0
3	D	816	0	0	10	1
All	All	26286	0	22516	144	2

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 3.

The worst 5 of 144 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:449[A]:HIS:CE1	3:A:1701:HOH:O	1.85	1.26
1:B:521:ARG:HD3	3:B:1548:HOH:O	1.37	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ARG:HH11	1:C:521:ARG:CG	1.46	1.19
1:D:451:MET:SD	3:D:1638:HOH:O	2.05	1.14
1:C:521:ARG:HG2	1:C:521:ARG:NH1	1.18	1.14

All (2) 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)
3:A:1596:HOH:O	3:D:1512:HOH:O[1_455]	1.99	0.21
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.10	0.10

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	727/753 (96%)	712 (98%)	14 (2%)	1 (0%)	56	35
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	39	20
1	C	729/753 (97%)	710 (97%)	17 (2%)	2 (0%)	46	26
1	D	727/753 (96%)	713 (98%)	13 (2%)	1 (0%)	56	35
All	All	2909/3012 (97%)	2841 (98%)	61 (2%)	7 (0%)	52	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	B	75	SER
1	A	75	SER
1	C	75	SER
1	C	725	ASP

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	614/635 (97%)	601 (98%)	13 (2%)	61	42
1	B	613/635 (96%)	590 (96%)	23 (4%)	40	17
1	C	616/635 (97%)	580 (94%)	36 (6%)	25	8
1	D	614/635 (97%)	597 (97%)	17 (3%)	51	29
All	All	2457/2540 (97%)	2368 (96%)	89 (4%)	42	19

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	PHE
1	C	440	TYR
1	D	554	LEU
1	C	191	THR
1	C	252	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	419	GLN
1	C	507	HIS
1	D	556	GLN
1	C	459	ASN
1	A	515	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](#)

4 non-standard protein/DNA/RNA residues 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
1	OCS	A	669	1	7,8,9	3.08	2 (28%)	7,11,13	2.93	2 (28%)
1	OCS	B	669	1	7,8,9	3.37	2 (28%)	7,11,13	3.84	2 (28%)
1	OCS	C	669	1	7,8,9	2.84	2 (28%)	7,11,13	1.25	1 (14%)
1	OCS	D	669	1	7,8,9	2.39	1 (14%)	7,11,13	2.60	3 (42%)

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
1	OCS	A	669	1	-	1/4/7/9	0/0/0/0
1	OCS	B	669	1	-	1/4/7/9	0/0/0/0
1	OCS	C	669	1	-	1/4/7/9	0/0/0/0
1	OCS	D	669	1	-	1/4/7/9	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	CB-SG	-4.64	1.71	1.77
1	C	669	OCS	CB-SG	-4.35	1.71	1.77
1	A	669	OCS	CB-SG	-2.01	1.75	1.77
1	D	669	OCS	OD2-SG	5.59	1.60	1.46
1	C	669	OCS	OD2-SG	5.86	1.61	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	669	OCS	OD3-SG-CB	-5.37	102.42	106.94
1	A	669	OCS	OD3-SG-CB	-2.91	104.49	106.94
1	B	669	OCS	OD3-SG-CB	-2.64	104.71	106.94
1	C	669	OCS	OD1-SG-CB	-2.32	104.99	106.94
1	D	669	OCS	OD2-SG-OD1	2.47	117.36	111.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	669	OCS	SG-CB-CA-N
1	D	669	OCS	SG-CB-CA-N
1	B	669	OCS	SG-CB-CA-N
1	A	669	OCS	SG-CB-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	669	OCS	1	0

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	HDD	A	801	1	30,52,52	1.84	8 (26%)	20,89,89	5.16	12 (60%)
2	HDD	B	801	1,3	30,52,52	1.71	7 (23%)	20,89,89	4.38	11 (55%)
2	HDD	C	801	1,3	30,52,52	1.81	7 (23%)	20,89,89	4.24	9 (45%)
2	HDD	D	801	1	30,52,52	1.63	5 (16%)	20,89,89	5.07	10 (50%)

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	HDD	A	801	1	-	0/3/89/89	0/1/9/9
2	HDD	B	801	1,3	-	0/3/89/89	0/1/9/9
2	HDD	C	801	1,3	-	0/3/89/89	0/1/9/9
2	HDD	D	801	1	-	0/3/89/89	0/1/9/9

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HDD	CAD-C3D	-2.46	1.48	1.53
2	B	801	HDD	C1D-ND	-2.43	1.34	1.38
2	D	801	HDD	C1A-CHA	2.00	1.45	1.39
2	B	801	HDD	C4A-CHB	2.08	1.45	1.39
2	C	801	HDD	O1D-CGD	2.18	1.39	1.35

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HDD	O1D-CGD-CBD	-12.17	95.94	110.20
2	D	801	HDD	O1D-CGD-CBD	-9.49	99.09	110.20
2	B	801	HDD	O1D-CGD-CBD	-8.52	100.22	110.20
2	B	801	HDD	OND-C2D-CMD	-8.27	94.47	109.41
2	C	801	HDD	OND-C2D-CMD	-7.65	95.60	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HDD	2	0
2	B	801	HDD	1	0
2	C	801	HDD	4	0
2	D	801	HDD	3	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 [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	725/753 (96%)	-0.48	5 (0%) 89 91	5, 11, 26, 54	1 (0%)
1	B	725/753 (96%)	-0.34	21 (2%) 55 59	5, 13, 36, 58	1 (0%)
1	C	725/753 (96%)	-0.38	20 (2%) 56 61	5, 12, 35, 54	1 (0%)
1	D	725/753 (96%)	-0.45	9 (1%) 81 85	5, 11, 28, 56	1 (0%)
All	All	2900/3012 (96%)	-0.41	55 (1%) 70 74	5, 12, 32, 58	4 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	5.1
1	B	28	SER	4.6
1	C	711	ALA	4.6
1	B	32	GLU	4.0
1	B	713	GLN	3.5

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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	C	669	9/10	0.93	0.16	-	27,31,41,44	0
1	OCS	D	669	9/10	0.94	0.13	-	19,23,28,38	0
1	OCS	A	669	9/10	0.91	0.12	-	16,20,31,38	0
1	OCS	B	669	9/10	0.92	0.15	-	29,31,40,46	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	HDD	A	801	44/44	0.99	0.07	0.38	5,6,13,16	0
2	HDD	D	801	44/44	0.99	0.07	0.29	5,6,12,16	0
2	HDD	C	801	44/44	0.99	0.07	0.21	6,7,15,18	0
2	HDD	B	801	44/44	0.99	0.07	0.02	6,7,13,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.