Full wwPDB X-ray Structure Validation Report (i)

May 15, 2024 – 07:02 PM EDT

PDB ID	:	2YAX
Title	:	IODOACETAMIDE INHIBITED SULFUR OXYGENASE REDUCTASE
Authors	:	Veith, A.; Urich, T.; Seyfarth, K.; Protze, J.; Frazao, C.; Kletzin, A.
Deposited on	:	2011-02-25
Resolution	:	1.80 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
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 (1)) were used in the production of this report:

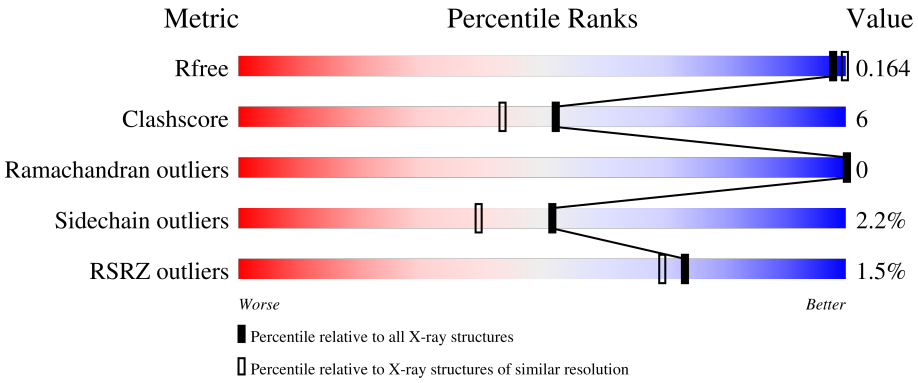
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	318	84% 11%
1	D	318	86% 10%
1	E	318	85% 10%
2	B	318	84% 11%
2	C	318	85% 10%

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Mol	Chain	Length	Quality of chain
2	F	318	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15532 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 SULFUR OXYGENASE/REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	12	0
			2517	1632	413	448	24			
1	D	307	Total	C	N	O	S	0	10	0
			2510	1628	411	448	23			
1	E	307	Total	C	N	O	S	0	8	0
			2500	1620	410	447	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	ASN	-	expression tag	UNP P29082
A	310	ALA	-	expression tag	UNP P29082
A	311	TRP	-	expression tag	UNP P29082
A	312	ARG	-	expression tag	UNP P29082
A	313	HIS	-	expression tag	UNP P29082
A	314	PRO	-	expression tag	UNP P29082
A	315	GLN	-	expression tag	UNP P29082
A	316	PHE	-	expression tag	UNP P29082
A	317	GLY	-	expression tag	UNP P29082
A	318	GLY	-	expression tag	UNP P29082
D	309	ASN	-	expression tag	UNP P29082
D	310	ALA	-	expression tag	UNP P29082
D	311	TRP	-	expression tag	UNP P29082
D	312	ARG	-	expression tag	UNP P29082
D	313	HIS	-	expression tag	UNP P29082
D	314	PRO	-	expression tag	UNP P29082
D	315	GLN	-	expression tag	UNP P29082
D	316	PHE	-	expression tag	UNP P29082
D	317	GLY	-	expression tag	UNP P29082
D	318	GLY	-	expression tag	UNP P29082
E	309	ASN	-	expression tag	UNP P29082
E	310	ALA	-	expression tag	UNP P29082
E	311	TRP	-	expression tag	UNP P29082

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Chain	Residue	Modelled	Actual	Comment	Reference
E	312	ARG	-	expression tag	UNP P29082
E	313	HIS	-	expression tag	UNP P29082
E	314	PRO	-	expression tag	UNP P29082
E	315	GLN	-	expression tag	UNP P29082
E	316	PHE	-	expression tag	UNP P29082
E	317	GLY	-	expression tag	UNP P29082
E	318	GLY	-	expression tag	UNP P29082

- Molecule 2 is a protein called SULFUR OXYGENASE/REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	9	0
			2504	1620	414	448	22			
2	C	307	Total	C	N	O	S	0	8	0
			2503	1622	413	447	21			
2	F	307	Total	C	N	O	S	0	12	0
			2515	1631	413	449	22			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	309	ASN	-	expression tag	UNP P29082
B	310	ALA	-	expression tag	UNP P29082
B	311	TRP	-	expression tag	UNP P29082
B	312	ARG	-	expression tag	UNP P29082
B	313	HIS	-	expression tag	UNP P29082
B	314	PRO	-	expression tag	UNP P29082
B	315	GLN	-	expression tag	UNP P29082
B	316	PHE	-	expression tag	UNP P29082
B	317	GLY	-	expression tag	UNP P29082
B	318	GLY	-	expression tag	UNP P29082
C	309	ASN	-	expression tag	UNP P29082
C	310	ALA	-	expression tag	UNP P29082
C	311	TRP	-	expression tag	UNP P29082
C	312	ARG	-	expression tag	UNP P29082
C	313	HIS	-	expression tag	UNP P29082
C	314	PRO	-	expression tag	UNP P29082
C	315	GLN	-	expression tag	UNP P29082
C	316	PHE	-	expression tag	UNP P29082
C	317	GLY	-	expression tag	UNP P29082
C	318	GLY	-	expression tag	UNP P29082
F	309	ASN	-	expression tag	UNP P29082

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Chain	Residue	Modelled	Actual	Comment	Reference
F	310	ALA	-	expression tag	UNP P29082
F	311	TRP	-	expression tag	UNP P29082
F	312	ARG	-	expression tag	UNP P29082
F	313	HIS	-	expression tag	UNP P29082
F	314	PRO	-	expression tag	UNP P29082
F	315	GLN	-	expression tag	UNP P29082
F	316	PHE	-	expression tag	UNP P29082
F	317	GLY	-	expression tag	UNP P29082
F	318	GLY	-	expression tag	UNP P29082

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is water.

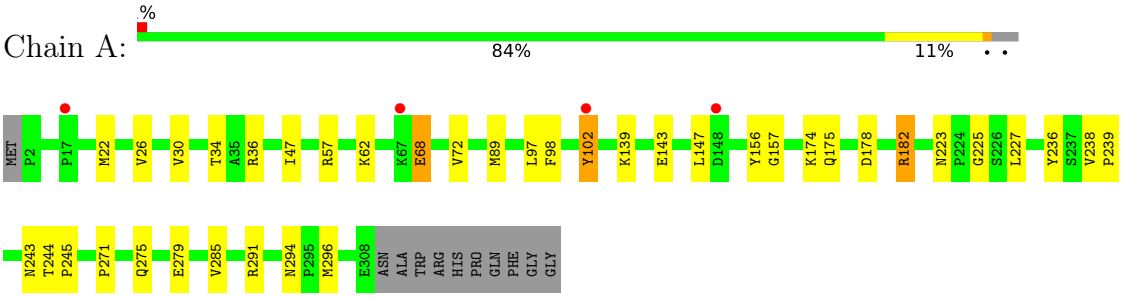
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total O 81 81	0	0
4	B	80	Total O 80 80	0	0
4	C	78	Total O 78 78	0	0
4	D	80	Total O 80 80	0	0
4	E	76	Total O 76 76	0	0
4	F	82	Total O 82 82	0	0

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.

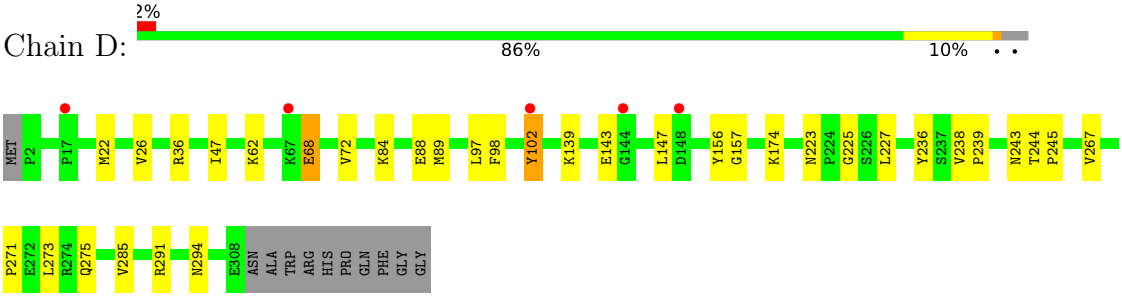
• Molecule 1: SULFUR OXYGENASE/REDUCTASE

Chain A:



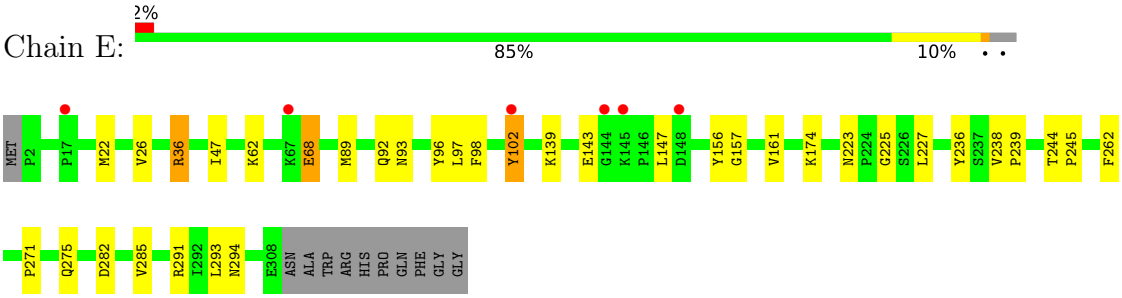
• Molecule 1: SULFUR OXYGENASE/REDUCTASE

Chain D:



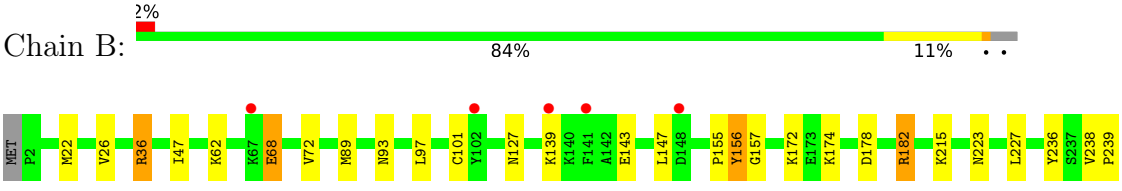
• Molecule 1: SULFUR OXYGENASE/REDUCTASE

Chain E:

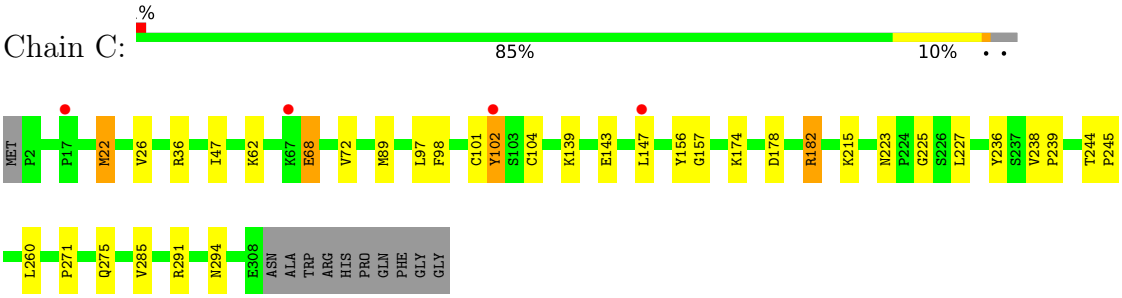


• Molecule 2: SULFUR OXYGENASE/REDUCTASE

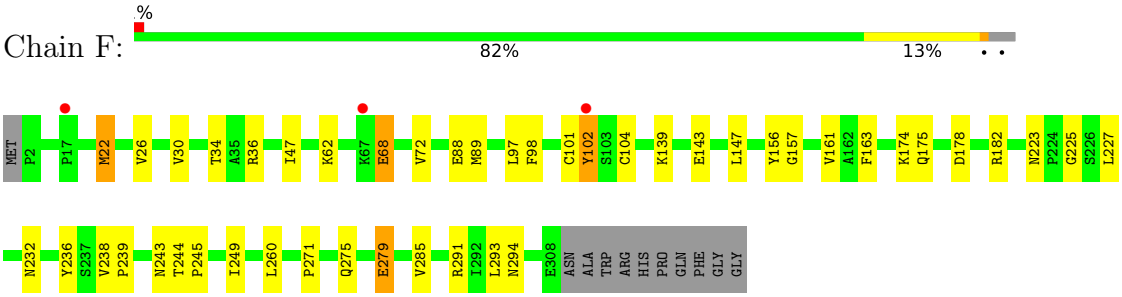
Chain B:



• Molecule 2: SULFUR OXYGENASE/REDUCTASE



• Molecule 2: SULFUR OXYGENASE/REDUCTASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	161.90Å 161.90Å 154.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.05 – 1.80 38.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.05-1.80) 94.4 (38.05-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.169 , 0.193 0.168 , 0.164	Depositor DCC
R_{free} test set	8668 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.002 for -l,-k,-h 0.005 for -h,-l,-k 0.000 for -h,l,k 0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15532	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, 0.333 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: FE, YCM, CSS

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	0.65	7/2631 (0.3%)	0.84	10/3563 (0.3%)
1	D	0.60	6/2615 (0.2%)	0.78	6/3542 (0.2%)
1	E	0.57	5/2597 (0.2%)	0.68	6/3518 (0.2%)
2	B	0.78	6/2594 (0.2%)	0.80	16/3512 (0.5%)
2	C	0.62	6/2593 (0.2%)	0.95	11/3512 (0.3%)
2	F	0.75	4/2621 (0.2%)	0.73	10/3550 (0.3%)
All	All	0.67	34/15651 (0.2%)	0.80	59/21197 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	156	TYR	CE2-CZ	-15.43	1.18	1.38
2	B	156	TYR	CE2-CZ	-15.09	1.19	1.38
2	B	156	TYR	CE1-CZ	-14.77	1.19	1.38
2	F	156	TYR	CE1-CZ	-14.49	1.19	1.38
2	F	156	TYR	CG-CD1	-14.47	1.20	1.39
2	B	156	TYR	CG-CD2	-14.07	1.20	1.39
2	F	156	TYR	CG-CD2	-13.47	1.21	1.39
2	B	156	TYR	CG-CD1	-12.96	1.22	1.39
1	A	57	ARG	CZ-NH2	-11.80	1.17	1.33
1	A	57	ARG	CZ-NH1	-11.75	1.17	1.33
2	C	291	ARG	CZ-NH2	-9.97	1.20	1.33
1	D	291	ARG	CZ-NH1	-9.74	1.20	1.33
1	D	291	ARG	CZ-NH2	-9.73	1.20	1.33
2	C	291	ARG	CZ-NH1	-9.43	1.20	1.33
2	B	127	ASN	CG-ND2	-8.64	1.11	1.32
2	C	156	TYR	CE1-CZ	-8.53	1.27	1.38
1	A	156	TYR	CE1-CZ	-8.30	1.27	1.38
2	B	127	ASN	CG-OD1	-8.25	1.05	1.24
2	C	156	TYR	CE2-CZ	-8.11	1.28	1.38
1	E	156	TYR	CE1-CZ	-7.99	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	TYR	CE2-CZ	-7.74	1.28	1.38
2	C	156	TYR	CG-CD2	-7.38	1.29	1.39
1	E	156	TYR	CE2-CZ	-7.37	1.28	1.38
1	E	156	TYR	CG-CD1	-7.27	1.29	1.39
1	D	156	TYR	CE2-CZ	-7.22	1.29	1.38
1	D	156	TYR	CG-CD2	-7.07	1.29	1.39
1	D	156	TYR	CE1-CZ	-7.03	1.29	1.38
2	C	156	TYR	CG-CD1	-6.90	1.30	1.39
1	E	156	TYR	CG-CD2	-6.85	1.30	1.39
1	A	156	TYR	CG-CD2	-6.67	1.30	1.39
1	A	156	TYR	CG-CD1	-6.14	1.31	1.39
1	D	156	TYR	CG-CD1	-6.03	1.31	1.39
1	A	291	ARG	CZ-NH2	-5.21	1.26	1.33
1	E	291	ARG	CZ-NH2	-5.03	1.26	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	ARG	NE-CZ-NH2	17.23	128.92	120.30
2	C	182[A]	ARG	NE-CZ-NH2	-17.01	111.80	120.30
2	C	182[B]	ARG	NE-CZ-NH2	-17.01	111.80	120.30
2	C	182[A]	ARG	NE-CZ-NH1	16.81	128.71	120.30
2	C	182[B]	ARG	NE-CZ-NH1	16.81	128.71	120.30
1	A	57	ARG	NE-CZ-NH1	15.26	127.93	120.30
1	A	57	ARG	NH1-CZ-NH2	-14.77	103.16	119.40
1	D	36	ARG	NE-CZ-NH1	14.41	127.50	120.30
2	B	36	ARG	NE-CZ-NH1	14.27	127.44	120.30
1	D	36	ARG	NE-CZ-NH2	-14.26	113.17	120.30
2	B	36	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	D	291	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	D	291	ARG	NE-CZ-NH1	12.61	126.60	120.30
2	C	291	ARG	NE-CZ-NH2	12.59	126.59	120.30
2	C	291	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	E	36	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	D	291	ARG	NH1-CZ-NH2	-11.49	106.77	119.40
2	C	291	ARG	NH1-CZ-NH2	-11.41	106.85	119.40
1	A	36	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	E	36	ARG	NE-CZ-NH1	9.92	125.26	120.30
2	C	36	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	A	36	ARG	NE-CZ-NH1	9.09	124.84	120.30
2	F	36	ARG	NE-CZ-NH2	-8.65	115.98	120.30
2	C	36	ARG	NE-CZ-NH1	8.38	124.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	36	ARG	NE-CZ-NH1	8.01	124.30	120.30
2	B	291	ARG	NE-CZ-NH1	7.71	124.16	120.30
2	C	182[A]	ARG	CD-NE-CZ	7.41	133.98	123.60
2	C	182[B]	ARG	CD-NE-CZ	7.41	133.98	123.60
2	B	156	TYR	CD1-CG-CD2	-7.40	109.76	117.90
2	B	156	TYR	CZ-CE2-CD2	7.36	126.42	119.80
1	A	291	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	B	156	TYR	CD1-CE1-CZ	7.32	126.39	119.80
2	F	156	TYR	CZ-CE2-CD2	7.09	126.19	119.80
2	F	156	TYR	CD1-CG-CD2	-7.03	110.17	117.90
2	F	156	TYR	CD1-CE1-CZ	6.94	126.05	119.80
2	B	156	TYR	CB-CG-CD1	6.91	125.15	121.00
2	F	156	TYR	CB-CG-CD2	6.83	125.10	121.00
2	B	36	ARG	CD-NE-CZ	6.78	133.09	123.60
2	B	156	TYR	CB-CG-CD2	6.77	125.06	121.00
2	B	156	TYR	CE1-CZ-CE2	-6.69	109.09	119.80
2	F	156	TYR	CE1-CZ-CE2	-6.52	109.37	119.80
1	D	36	ARG	CD-NE-CZ	6.33	132.47	123.60
1	E	291	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	F	156	TYR	CB-CG-CD1	6.14	124.69	121.00
2	B	182[A]	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	B	182[B]	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	B	291	ARG	NH1-CZ-NH2	-5.99	112.81	119.40
1	A	291	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
2	F	279	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	E	291	ARG	NE-CZ-NH2	5.57	123.08	120.30
2	B	291	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	E	291	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	E	36	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	291	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	182[A]	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	182[B]	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	182[A]	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	182[B]	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	F	291	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	2517	0	2475	32	0
1	D	2510	0	2464	28	0
1	E	2500	0	2451	30	2
2	B	2504	0	2457	20	1
2	C	2503	0	2457	30	1
2	F	2515	0	2471	35	2
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	81	0	0	1	0
4	B	80	0	0	1	0
4	C	78	0	0	0	0
4	D	80	0	0	0	0
4	E	76	0	0	2	0
4	F	82	0	0	1	0
All	All	15532	0	14775	166	3

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.

All (166) 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:139:LYS:O	2:B:143:GLU:HG3	1.78	0.84
1:E:139:LYS:O	1:E:143:GLU:HG3	1.77	0.84
1:D:139:LYS:O	1:D:143:GLU:HG3	1.77	0.83
1:A:139:LYS:O	1:A:143:GLU:HG3	1.79	0.81
2:C:139:LYS:O	2:C:143:GLU:HG3	1.80	0.81
2:F:30:VAL:O	2:F:34[A]:THR:HG23	1.82	0.80
1:A:30:VAL:O	1:A:34[A]:THR:HG23	1.82	0.80
2:C:102[B]:TYR:CD2	2:C:225:GLY:HA2	2.17	0.80
1:D:102[B]:TYR:CD2	1:D:225:GLY:HA2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:LYS:O	2:F:143:GLU:HG3	1.84	0.76
1:D:102[B]:TYR:CE2	1:D:225:GLY:HA2	2.22	0.74
2:C:102[B]:TYR:CE2	2:C:225:GLY:HA2	2.21	0.74
1:A:102[B]:TYR:CD2	1:A:225:GLY:HA2	2.23	0.73
1:A:178[B]:ASP:OD2	1:A:182[B]:ARG:NH1	2.21	0.73
2:F:102[B]:TYR:CD2	2:F:225:GLY:HA2	2.23	0.73
1:E:102[B]:TYR:CD2	1:E:225:GLY:HA2	2.25	0.72
2:F:178[B]:ASP:OD2	2:F:182[B]:ARG:NH1	2.24	0.70
2:B:178[B]:ASP:OD2	2:B:182[B]:ARG:NH1	2.24	0.70
1:E:102[B]:TYR:CE2	1:E:225:GLY:HA2	2.28	0.67
1:A:102[B]:TYR:CE2	1:A:225:GLY:HA2	2.29	0.66
2:F:102[B]:TYR:CE2	2:F:225:GLY:HA2	2.29	0.66
2:C:62:LYS:HE2	2:C:68:GLU:OE2	1.96	0.66
2:F:102[A]:TYR:CE2	2:F:223:ASN:HB3	2.31	0.65
2:F:102[A]:TYR:HE2	2:F:223:ASN:HB3	1.61	0.65
1:D:102[A]:TYR:CE2	1:D:223:ASN:HB3	2.31	0.64
1:A:102[A]:TYR:CE2	1:A:223:ASN:HB3	2.32	0.64
1:D:102[A]:TYR:HE2	1:D:223:ASN:HB3	1.63	0.64
1:A:62:LYS:HE2	1:A:68:GLU:OE2	1.97	0.63
1:D:62:LYS:HE2	1:D:68:GLU:OE2	1.97	0.63
1:E:102[A]:TYR:HE2	1:E:223:ASN:HB3	1.64	0.63
1:E:62:LYS:HE2	1:E:68:GLU:OE2	1.98	0.63
1:A:102[A]:TYR:HE2	1:A:223:ASN:HB3	1.63	0.63
2:B:62:LYS:HE2	2:B:68:GLU:OE2	1.99	0.63
1:A:34[B]:THR:HG22	1:A:89:MET:CE	2.30	0.62
2:C:102[A]:TYR:CE2	2:C:223:ASN:HB3	2.35	0.61
1:E:102[A]:TYR:CE2	1:E:223:ASN:HB3	2.35	0.61
2:C:178[B]:ASP:OD2	2:C:182[B]:ARG:NH2	2.34	0.60
2:F:182[B]:ARG:NH2	2:F:279:GLU:OE1	2.34	0.60
1:E:96:TYR:CE2	4:E:2003:HOH:O	2.54	0.60
2:F:34[B]:THR:HG22	2:F:89:MET:CE	2.31	0.60
2:C:102[A]:TYR:HE2	2:C:223:ASN:HB3	1.65	0.59
2:F:62:LYS:HE2	2:F:68:GLU:OE2	2.03	0.59
1:E:96:TYR:CZ	4:E:2003:HOH:O	2.51	0.57
2:B:47[A]:ILE:HG23	2:B:72:VAL:CG2	2.37	0.54
2:B:155:PRO:HB2	2:B:156:TYR:CD2	2.43	0.53
1:A:47[A]:ILE:HG23	1:A:72:VAL:CG2	2.39	0.53
1:A:98:PHE:CZ	1:A:102[A]:TYR:HD2	2.27	0.53
2:C:271:PRO:O	2:C:275:GLN:HG2	2.09	0.53
1:A:182[B]:ARG:NH2	1:A:279:GLU:OE1	2.42	0.53
1:E:98:PHE:CZ	1:E:102[A]:TYR:HD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47[A]:ILE:HG23	2:C:72:VAL:CG2	2.39	0.53
1:D:47[A]:ILE:HG23	1:D:72:VAL:CG2	2.39	0.53
2:C:22:MET:SD	2:C:104:CYS:SG	3.02	0.53
2:C:223:ASN:ND2	2:C:227:LEU:O	2.35	0.53
2:F:47[A]:ILE:HG23	2:F:72:VAL:CG2	2.38	0.53
2:F:223:ASN:ND2	2:F:227:LEU:O	2.35	0.52
2:F:98:PHE:CZ	2:F:102[A]:TYR:HD2	2.26	0.52
2:C:102[B]:TYR:CE2	2:C:225:GLY:CA	2.90	0.52
2:B:238:VAL:HB	2:B:239:PRO:HD3	1.93	0.51
1:D:98:PHE:CZ	1:D:102[A]:TYR:HD2	2.28	0.51
2:F:271:PRO:O	2:F:275:GLN:HG2	2.11	0.51
1:A:271:PRO:O	1:A:275:GLN:HG2	2.12	0.50
2:F:89:MET:SD	2:F:97:LEU:HD11	2.51	0.50
2:C:98:PHE:CZ	2:C:102[A]:TYR:HD2	2.29	0.50
2:F:238:VAL:HB	2:F:239:PRO:HD3	1.94	0.50
1:D:236:TYR:CE1	2:F:285:VAL:HA	2.47	0.50
1:D:102[B]:TYR:CE2	1:D:225:GLY:CA	2.92	0.50
1:D:271:PRO:O	1:D:275:GLN:HG2	2.12	0.50
1:E:89:MET:SD	1:E:97:LEU:HD11	2.52	0.50
2:C:89:MET:SD	2:C:97:LEU:HD11	2.52	0.49
1:D:285:VAL:HA	2:F:236:TYR:CE1	2.47	0.49
1:A:238:VAL:HB	1:A:239:PRO:HD3	1.94	0.49
1:E:271:PRO:O	1:E:275:GLN:HG2	2.12	0.49
1:A:89:MET:SD	1:A:97:LEU:HD11	2.52	0.49
2:B:271:PRO:O	2:B:275:GLN:HG2	2.13	0.48
2:C:285:VAL:HA	1:E:236:TYR:CE1	2.49	0.48
1:E:238:VAL:HB	1:E:239:PRO:HD3	1.96	0.47
2:C:236:TYR:CE1	1:E:285:VAL:HA	2.49	0.47
1:D:89:MET:SD	1:D:97:LEU:HD11	2.55	0.47
2:F:22:MET:SD	2:F:104:CYS:SG	3.10	0.47
1:A:285:VAL:HA	2:B:236:TYR:CE1	2.50	0.47
2:B:182[B]:ARG:NH2	2:B:279:GLU:OE1	2.48	0.47
1:A:236:TYR:CE1	2:B:285:VAL:HA	2.49	0.46
2:F:102[B]:TYR:CE2	2:F:225:GLY:CA	2.97	0.46
1:A:102[B]:TYR:CE2	1:A:225:GLY:CA	2.97	0.46
2:B:89:MET:SD	2:B:97:LEU:HD11	2.56	0.45
2:B:172:LYS:HE3	4:B:2075:HOH:O	2.17	0.45
2:C:22:MET:CE	2:C:104:CYS:SG	3.04	0.45
1:E:157:GLY:HA2	1:E:294:ASN:OD1	2.17	0.45
2:C:238:VAL:HB	2:C:239:PRO:HD3	1.98	0.44
2:F:175:GLN:HG3	4:F:2042:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:GLY:HA2	2:F:294:ASN:OD1	2.18	0.44
1:E:102[B]:TYR:CE2	1:E:225:GLY:CA	2.99	0.44
1:D:238:VAL:HB	1:D:239:PRO:HD3	2.00	0.44
1:D:243[B]:ASN:OD1	2:F:243[B]:ASN:ND2	2.38	0.44
1:A:157:GLY:HA2	1:A:294:ASN:OD1	2.18	0.43
2:C:157:GLY:HA2	2:C:294:ASN:OD1	2.17	0.43
2:B:155:PRO:HB2	2:B:156:TYR:CE2	2.52	0.43
2:C:244:THR:HA	2:C:245:PRO:C	2.39	0.43
1:A:243[B]:ASN:ND2	2:B:243[B]:ASN:OD1	2.43	0.43
2:C:260:LEU:HD23	2:C:260:LEU:C	2.39	0.43
1:D:244:THR:HA	1:D:245:PRO:C	2.40	0.42
2:B:157:GLY:HA2	2:B:294:ASN:OD1	2.19	0.42
2:B:244:THR:HA	2:B:245:PRO:C	2.40	0.42
1:E:47:ILE:O	1:E:47:ILE:HG13	2.18	0.42
2:B:267:VAL:HA	2:B:273:LEU:HG	2.02	0.42
2:B:156:TYR:CE1	1:E:262:PHE:HB2	2.55	0.42
1:A:175:GLN:HG3	4:A:2074:HOH:O	2.19	0.42
1:A:244:THR:HA	1:A:245:PRO:C	2.40	0.42
1:A:223:ASN:ND2	1:A:227:LEU:O	2.37	0.41
2:B:223:ASN:ND2	2:B:227:LEU:O	2.41	0.41
2:F:244:THR:HA	2:F:245:PRO:C	2.40	0.41
2:C:22:MET:HE3	2:C:104:CYS:SG	2.60	0.41
1:D:267:VAL:HA	1:D:273:LEU:HG	2.03	0.41
2:F:163:PHE:CE2	2:F:249[A]:ILE:HD13	2.55	0.41
1:D:157:GLY:HA2	1:D:294:ASN:OD1	2.20	0.41
1:E:244:THR:HA	1:E:245:PRO:C	2.41	0.41
1:E:223:ASN:ND2	1:E:227:LEU:O	2.37	0.41
1:A:47[A]:ILE:HD12	1:A:296[A]:MET:SD	2.61	0.41
1:D:223:ASN:ND2	1:D:227:LEU:O	2.40	0.41
2:F:260:LEU:C	2:F:260:LEU:HD23	2.41	0.41
2:B:36:ARG:HD3	2:B:93:ASN:OD1	2.20	0.41
1:E:161:VAL:HB	1:E:293:LEU:HB2	2.04	0.40
1:D:84:LYS:O	1:D:88[B]:GLU:HG3	2.22	0.40
1:E:36:ARG:HD3	1:E:93:ASN:OD1	2.22	0.40
2:F:161:VAL:HB	2:F:293:LEU:HB2	2.02	0.40

All (3) 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:215:LYS:NZ	1:E:92:GLN:NE2[6_564]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:LYS:NZ	2:F:232:ASN:OD1[6_564]	2.09	0.11
1:E:282:ASP:OD2	2:F:88:GLU:OE2[6_564]	2.19	0.01

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	316/318 (99%)	310 (98%)	6 (2%)	0	100	100
1	D	314/318 (99%)	308 (98%)	6 (2%)	0	100	100
1	E	312/318 (98%)	305 (98%)	7 (2%)	0	100	100
2	B	312/318 (98%)	306 (98%)	6 (2%)	0	100	100
2	C	311/318 (98%)	305 (98%)	6 (2%)	0	100	100
2	F	315/318 (99%)	308 (98%)	7 (2%)	0	100	100
All	All	1880/1908 (98%)	1842 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	276/272 (102%)	268 (97%)	8 (3%)	42	29
1	D	274/272 (101%)	266 (97%)	8 (3%)	42	29
1	E	272/272 (100%)	264 (97%)	8 (3%)	42	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	272/271 (100%)	266 (98%)	6 (2%)	52 39
2	C	271/271 (100%)	264 (97%)	7 (3%)	46 32
2	F	275/271 (102%)	268 (98%)	7 (2%)	47 34
All	All	1640/1629 (101%)	1596 (97%)	44 (3%)	52 31

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	MET
1	A	22[B]	MET
1	A	26	VAL
1	A	68	GLU
1	A	102[A]	TYR
1	A	102[B]	TYR
1	A	147	LEU
1	A	174	LYS
2	B	22[A]	MET
2	B	22[B]	MET
2	B	26	VAL
2	B	68	GLU
2	B	147	LEU
2	B	174	LYS
2	C	22	MET
2	C	26	VAL
2	C	68	GLU
2	C	102[A]	TYR
2	C	102[B]	TYR
2	C	147	LEU
2	C	174	LYS
1	D	22[A]	MET
1	D	22[B]	MET
1	D	26	VAL
1	D	68	GLU
1	D	102[A]	TYR
1	D	102[B]	TYR
1	D	147	LEU
1	D	174	LYS
1	E	22[A]	MET
1	E	22[B]	MET
1	E	26	VAL
1	E	68	GLU

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Mol	Chain	Res	Type
1	E	102[A]	TYR
1	E	102[B]	TYR
1	E	147	LEU
1	E	174	LYS
2	F	22	MET
2	F	26	VAL
2	F	68	GLU
2	F	102[A]	TYR
2	F	102[B]	TYR
2	F	147	LEU
2	F	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	76	GLN
1	A	127	ASN
1	A	247	GLN
2	B	9	ASN
2	B	76	GLN
2	B	247	GLN
2	C	9	ASN
2	C	76	GLN
2	C	127	ASN
2	C	247	GLN
1	D	9	ASN
1	D	127	ASN
1	D	247	GLN
1	E	9	ASN
1	E	76	GLN
1	E	127	ASN
1	E	247	GLN
2	F	9	ASN
2	F	76	GLN
2	F	127	ASN
2	F	247	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

9 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	CSS	E	31	1	4,6,7	1.05	0	1,6,8	0.65	0
2	CSS	B	31	2	4,6,7	1.34	0	1,6,8	0.72	0
2	YCM	F	101	2	7,9,10	1.64	2 (28%)	4,10,12	0.91	0
2	CSS	C	31	2	4,6,7	1.10	0	1,6,8	1.05	0
2	YCM	C	101	2	7,9,10	1.76	1 (14%)	4,10,12	1.88	1 (25%)
2	YCM	B	101	2	7,9,10	1.60	1 (14%)	4,10,12	0.92	0
1	CSS	D	31	1	4,6,7	1.17	0	1,6,8	0.74	0
2	CSS	F	31	2	4,6,7	1.15	0	1,6,8	0.32	0
1	CSS	A	31	1	4,6,7	1.09	0	1,6,8	0.68	0

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	CSS	E	31	1	-	0/1/5/7	-
2	CSS	B	31	2	-	0/1/5/7	-
2	YCM	F	101	2	-	1/6/8/10	-
2	CSS	C	31	2	-	0/1/5/7	-
2	YCM	C	101	2	-	6/6/8/10	-
2	YCM	B	101	2	-	2/6/8/10	-
1	CSS	D	31	1	-	0/1/5/7	-
2	CSS	F	31	2	-	0/1/5/7	-
1	CSS	A	31	1	-	0/1/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101	YCM	CE-NZ2	3.90	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	YCM	CE-NZ2	3.70	1.44	1.32
2	F	101	YCM	CE-NZ2	3.64	1.44	1.32
2	F	101	YCM	O-C	2.02	1.28	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	101	YCM	CA-CB-SG	-3.21	101.98	113.74

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	101	YCM	SG-CD-CE-OZ1
2	B	101	YCM	SG-CD-CE-NZ2
2	C	101	YCM	N-CA-CB-SG
2	C	101	YCM	C-CA-CB-SG
2	C	101	YCM	CA-CB-SG-CD
2	C	101	YCM	CE-CD-SG-CB
2	C	101	YCM	SG-CD-CE-OZ1
2	C	101	YCM	SG-CD-CE-NZ2
2	F	101	YCM	SG-CD-CE-NZ2

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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	306/318 (96%)	-0.30	4 (1%)	77	74	23, 29, 48, 68	0
1	D	306/318 (96%)	-0.33	5 (1%)	72	68	23, 29, 49, 68	0
1	E	306/318 (96%)	-0.32	6 (1%)	65	61	23, 29, 49, 67	0
2	B	305/318 (95%)	-0.29	5 (1%)	72	68	24, 29, 50, 67	0
2	C	305/318 (95%)	-0.27	4 (1%)	77	74	24, 29, 49, 68	0
2	F	305/318 (95%)	-0.26	3 (0%)	82	80	21, 29, 48, 68	0
All	All	1833/1908 (96%)	-0.30	27 (1%)	73	70	21, 29, 50, 68	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	102[A]	TYR	7.8
1	E	102[A]	TYR	6.6
1	A	102[A]	TYR	6.1
2	C	102[A]	TYR	5.9
1	D	102[A]	TYR	5.6
1	A	67	LYS	3.7
2	F	67	LYS	3.1
2	C	17	PRO	2.9
1	A	17	PRO	2.8
1	D	144	GLY	2.7
1	E	145	LYS	2.7
2	C	67	LYS	2.7
1	D	67	LYS	2.7
2	B	67	LYS	2.5
2	C	147	LEU	2.5
1	D	148	ASP	2.4
1	E	148	ASP	2.4
2	B	141	PHE	2.4
1	E	17	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	17	PRO	2.3
2	F	17	PRO	2.2
2	B	148	ASP	2.2
1	E	67	LYS	2.2
2	B	139	LYS	2.2
1	E	144	GLY	2.1
2	B	102	TYR	2.1
1	A	148	ASP	2.1

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, 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	B-factors(Å^2)	Q<0.9
2	YCM	F	101	10/11	0.84	0.14	43,54,80,84	0
2	YCM	B	101	10/11	0.86	0.19	45,53,80,84	0
2	YCM	C	101	10/11	0.88	0.14	41,58,81,95	0
2	CSS	F	31	7/8	0.92	0.09	27,29,41,64	0
1	CSS	D	31	7/8	0.92	0.08	27,29,43,71	0
1	CSS	A	31	7/8	0.93	0.07	26,29,43,72	0
1	CSS	E	31	7/8	0.93	0.07	29,30,45,64	0
2	CSS	B	31	7/8	0.95	0.06	28,29,44,61	0
2	CSS	C	31	7/8	0.97	0.06	32,33,47,76	0

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, 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	B-factors(Å^2)	Q<0.9
3	FE	A	1309	1/1	0.99	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	D	1309	1/1	0.99	0.05	34,34,34,34	0
3	FE	E	1309	1/1	0.99	0.06	33,33,33,33	0
3	FE	B	1309	1/1	1.00	0.04	33,33,33,33	0
3	FE	C	1309	1/1	1.00	0.03	34,34,34,34	0
3	FE	F	1309	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.