Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2024 – 01:26 pm GMT

PDB ID	:	8QKE
Title	:	PvSub1 Catalytic Domain in Complex with Peptidomimetic Inhibitor (MH-13)
Authors	:	Batista, F.A.; Martinez, M.; Bouillon, A.; Mechaly, A.; Alzari, P.M.; Haouz, A.; Barale, J.C.
Deposited on	:	2023-09-15
Resolution	:	1.50 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 ⓘ 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 ⓘ) were used in the production of this report:

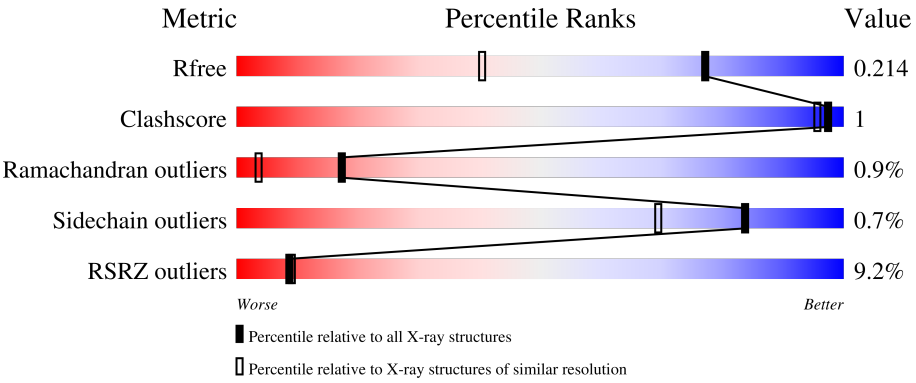
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	631	5% 51% · 47%
1	B	631	5% 52% · 47%
2	C	7	71% 29%
2	D	7	14% 71% 29%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5698 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 subtilisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2582	1619	455	496	12			
1	B	336	Total	C	N	O	S	0	0	0
			2603	1631	458	502	12			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP E6Y8B9
A	7	LYS	-	expression tag	UNP E6Y8B9
A	8	LEU	-	expression tag	UNP E6Y8B9
A	9	CYS	-	expression tag	UNP E6Y8B9
A	10	ILE	-	expression tag	UNP E6Y8B9
A	11	LEU	-	expression tag	UNP E6Y8B9
A	12	LEU	-	expression tag	UNP E6Y8B9
A	13	ALA	-	expression tag	UNP E6Y8B9
A	14	VAL	-	expression tag	UNP E6Y8B9
A	15	VAL	-	expression tag	UNP E6Y8B9
A	16	ALA	-	expression tag	UNP E6Y8B9
A	17	PHE	-	expression tag	UNP E6Y8B9
A	18	VAL	-	expression tag	UNP E6Y8B9
A	19	GLY	-	expression tag	UNP E6Y8B9
A	20	LEU	-	expression tag	UNP E6Y8B9
A	21	SER	-	expression tag	UNP E6Y8B9
A	22	LEU	-	expression tag	UNP E6Y8B9
A	23	GLY	-	expression tag	UNP E6Y8B9
A	24	ARG	-	expression tag	UNP E6Y8B9
A	25	SER	-	expression tag	UNP E6Y8B9
A	361	SER	ASN	engineered mutation	UNP E6Y8B9
A	432	SER	ASN	engineered mutation	UNP E6Y8B9
A	445	SER	ASN	engineered mutation	UNP E6Y8B9
A	631	HIS	-	expression tag	UNP E6Y8B9
A	632	HIS	-	expression tag	UNP E6Y8B9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	633	HIS	-	expression tag	UNP E6Y8B9
A	634	HIS	-	expression tag	UNP E6Y8B9
A	635	HIS	-	expression tag	UNP E6Y8B9
A	636	HIS	-	expression tag	UNP E6Y8B9
B	6	MET	-	initiating methionine	UNP E6Y8B9
B	7	LYS	-	expression tag	UNP E6Y8B9
B	8	LEU	-	expression tag	UNP E6Y8B9
B	9	CYS	-	expression tag	UNP E6Y8B9
B	10	ILE	-	expression tag	UNP E6Y8B9
B	11	LEU	-	expression tag	UNP E6Y8B9
B	12	LEU	-	expression tag	UNP E6Y8B9
B	13	ALA	-	expression tag	UNP E6Y8B9
B	14	VAL	-	expression tag	UNP E6Y8B9
B	15	VAL	-	expression tag	UNP E6Y8B9
B	16	ALA	-	expression tag	UNP E6Y8B9
B	17	PHE	-	expression tag	UNP E6Y8B9
B	18	VAL	-	expression tag	UNP E6Y8B9
B	19	GLY	-	expression tag	UNP E6Y8B9
B	20	LEU	-	expression tag	UNP E6Y8B9
B	21	SER	-	expression tag	UNP E6Y8B9
B	22	LEU	-	expression tag	UNP E6Y8B9
B	23	GLY	-	expression tag	UNP E6Y8B9
B	24	ARG	-	expression tag	UNP E6Y8B9
B	25	SER	-	expression tag	UNP E6Y8B9
B	361	SER	ASN	engineered mutation	UNP E6Y8B9
B	432	SER	ASN	engineered mutation	UNP E6Y8B9
B	445	SER	ASN	engineered mutation	UNP E6Y8B9
B	631	HIS	-	expression tag	UNP E6Y8B9
B	632	HIS	-	expression tag	UNP E6Y8B9
B	633	HIS	-	expression tag	UNP E6Y8B9
B	634	HIS	-	expression tag	UNP E6Y8B9
B	635	HIS	-	expression tag	UNP E6Y8B9
B	636	HIS	-	expression tag	UNP E6Y8B9

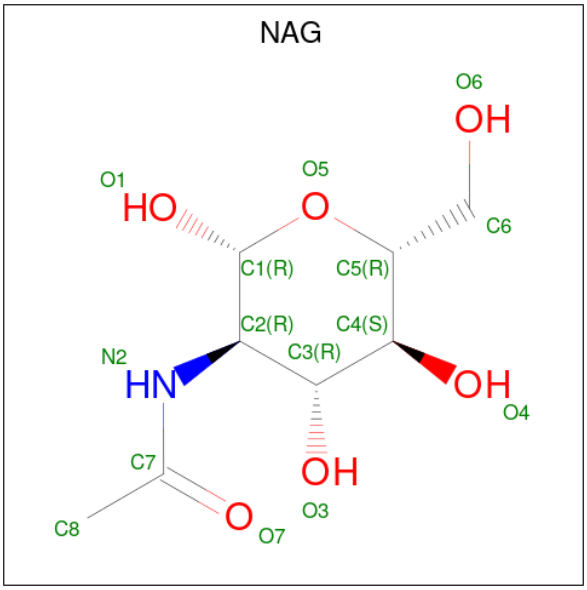
- Molecule 2 is a protein called Peptidomimetic Inhibitor (MH-13).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			44	27	6	11			
2	D	7	Total	C	N	O	0	0	0
			44	27	6	11			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

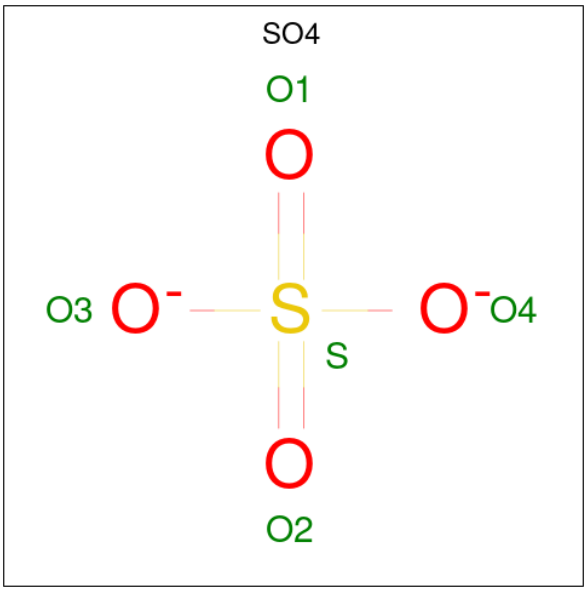
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	B	3	Total Ca 3 3	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

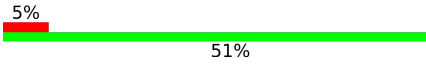
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	209	Total O 209 209	0	0
6	B	181	Total O 181 181	0	0
6	C	3	Total O 3 3	0	0
6	D	2	Total O 2 2	0	0

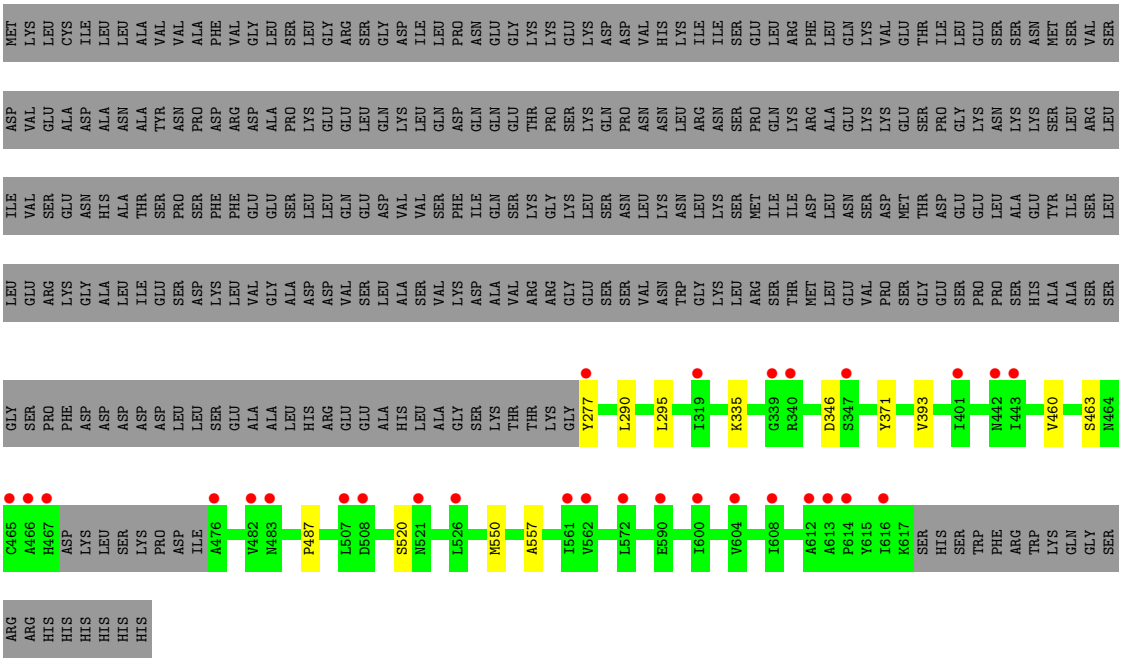
3 Residue-property plots (i)

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: subtilisin

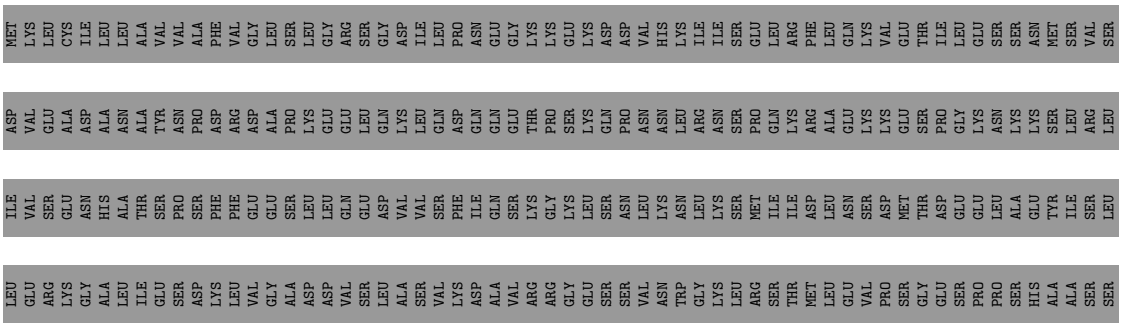
Chain A:

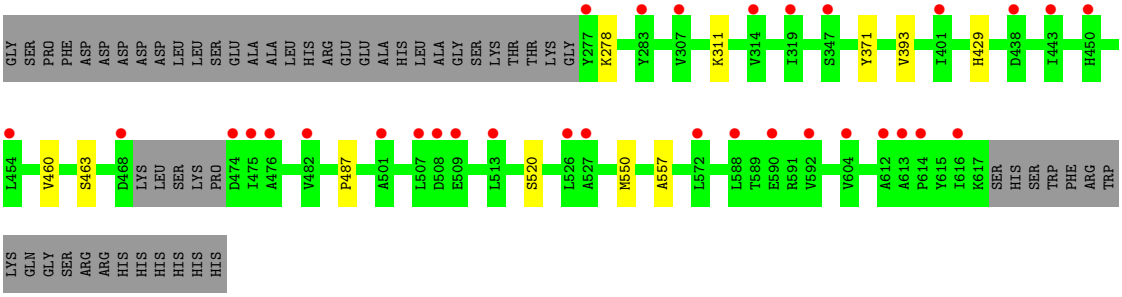




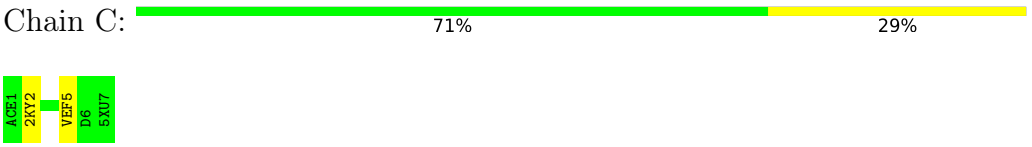
• Molecule 1: subtilisin

Chain B:

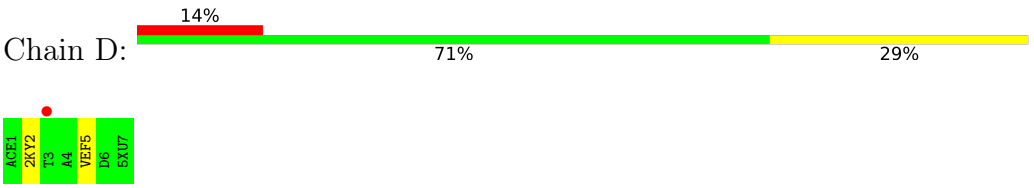




• Molecule 2: Peptidomimetic Inhibitor (MH-13)



• Molecule 2: Peptidomimetic Inhibitor (MH-13)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.02Å 54.71Å 69.14Å 69.39° 78.52° 75.02°	Depositor
Resolution (Å)	21.65 – 1.50 21.65 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (21.65-1.50) 94.3 (21.65-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.50Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.209 , 0.226 0.199 , 0.214	Depositor DCC
R_{free} test set	5232 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5698	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, VEF, 2KY, ACE, CA, NAG, 5XU

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	0.45	0/2634	0.58	0/3575
1	B	0.42	0/2652	0.57	0/3600
2	C	0.37	0/18	0.63	0/22
2	D	0.38	0/18	0.85	0/22
All	All	0.43	0/5322	0.57	0/7219

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
2	C	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	5	VEF	Mainchain,Peptide
2	D	5	VEF	Mainchain,Peptide

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	2582	0	2528	4	0
1	B	2603	0	2543	4	0
2	C	44	0	25	0	0
2	D	44	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	14	0	13	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	209	0	0	0	0
6	B	181	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
All	All	5698	0	5133	8	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 1.

All (8) 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:B:311:LYS:H	1:B:429:HIS:HD2	1.26	0.81
1:B:311:LYS:H	1:B:429:HIS:CD2	2.15	0.53
1:B:460:VAL:HG21	1:B:487:PRO:HD2	1.96	0.48
1:A:460:VAL:HG21	1:A:487:PRO:HD2	1.97	0.47
1:A:393:VAL:HB	1:A:557:ALA:CB	2.48	0.43
1:A:290:LEU:HD22	1:A:295:LEU:HD22	2.00	0.42
1:B:393:VAL:HB	1:B:557:ALA:CB	2.50	0.42
1:A:335:LYS:HB2	1:A:346:ASP:HB3	2.03	0.41

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	330/631 (52%)	320 (97%)	7 (2%)	3 (1%)	17 3
1	B	332/631 (53%)	319 (96%)	10 (3%)	3 (1%)	17 3
2	C	3/7 (43%)	3 (100%)	0	0	100 100
2	D	3/7 (43%)	3 (100%)	0	0	100 100
All	All	668/1276 (52%)	645 (97%)	17 (2%)	6 (1%)	17 3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	TYR
1	B	371	TYR
1	A	520	SER
1	B	520	SER
1	A	463	SER
1	B	463	SER

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	288/551 (52%)	286 (99%)	2 (1%)	84 69
1	B	290/551 (53%)	288 (99%)	2 (1%)	84 69
2	C	2/2 (100%)	2 (100%)	0	100 100
2	D	2/2 (100%)	2 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	582/1106 (53%)	578 (99%)	4 (1%)	84 69

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	TYR
1	A	550	MET
1	B	278	LYS
1	B	550	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	HIS
1	A	516	ASN
1	B	285	ASN
1	B	429	HIS
1	B	484	HIS
1	B	516	ASN
1	B	532	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)

6 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	$\#\|Z\| > 2$
2	5XU	D	7	2	3,4,4	0.36	0	2,4,4	0.44	0
2	5XU	C	7	2	3,4,4	0.33	0	2,4,4	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	2KY	C	2	2	8,9,10	0.50	0	6,11,13	1.11	1 (16%)
2	2KY	D	2	2	8,9,10	0.52	0	6,11,13	1.17	1 (16%)
2	VEF	C	5	2,1	4,6,8	0.56	0	3,7,12	0.82	0
2	VEF	D	5	2,1	4,6,8	0.49	0	3,7,12	0.60	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
2	5XU	D	7	2	-	0/0/2/2	-
2	5XU	C	7	2	-	0/0/2/2	-
2	2KY	C	2	2	-	2/3/13/15	0/1/1/1
2	2KY	D	2	2	-	2/3/13/15	0/1/1/1
2	VEF	C	5	2,1	-	0/5/6/12	-
2	VEF	D	5	2,1	-	0/5/6/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	2KY	C35-C34-C33	-2.22	98.83	104.96
2	C	2	2KY	C35-C34-C33	-2.16	98.97	104.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	2KY	C34-C33-CA-C
2	C	2	2KY	C37-C33-CA-C
2	D	2	2KY	C34-C33-CA-C
2	D	2	2KY	C37-C33-CA-C

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	SO4	B	904	-	4,4,4	0.17	0	6,6,6	0.37	0
5	SO4	A	905	-	4,4,4	0.20	0	6,6,6	0.40	0
4	NAG	A	904	1	14,14,15	0.30	0	17,19,21	0.61	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
4	NAG	A	904	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	904	NAG	C8-C7-N2-C2
4	A	904	NAG	O7-C7-N2-C2

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	333/631 (52%)	0.66	29 (8%) 10 10	19, 26, 40, 52	0
1	B	336/631 (53%)	0.77	32 (9%) 8 8	21, 29, 44, 60	0
2	C	3/7 (42%)	0.47	0 100 100	24, 24, 28, 35	0
2	D	3/7 (42%)	0.86	1 (33%) 0 0	27, 27, 32, 40	0
All	All	675/1276 (52%)	0.71	62 (9%) 9 9	19, 28, 43, 60	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	TYR	13.9
1	B	277	TYR	12.7
1	B	507	LEU	9.9
1	B	509	GLU	7.5
1	A	507	LEU	7.3
1	B	468	ASP	6.1
1	B	508	ASP	5.0
1	B	443	ILE	4.2
1	A	466	ALA	3.8
1	A	319	ILE	3.7
1	A	401	ILE	3.5
1	A	508	ASP	3.5
1	B	401	ILE	3.4
1	A	443	ILE	3.4
1	A	482	VAL	3.3
1	B	347	SER	3.3
1	B	612	ALA	3.3
1	A	590	GLU	3.2
1	A	476	ALA	3.2
1	A	612	ALA	3.2
1	B	526	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	482	VAL	3.0
1	A	604	VAL	2.9
1	B	616	ILE	2.9
1	B	475	ILE	2.7
1	B	307	VAL	2.7
1	B	613	ALA	2.6
1	A	339	GLY	2.6
1	B	614	PRO	2.6
1	B	474	ASP	2.6
1	B	476	ALA	2.5
1	A	521	ASN	2.5
1	B	592	VAL	2.5
1	A	600	ILE	2.5
1	B	319	ILE	2.5
1	A	467	HIS	2.4
2	D	3	THR	2.4
1	B	527	ALA	2.4
1	A	616	ILE	2.4
1	B	590	GLU	2.4
1	B	314	VAL	2.4
1	B	588	LEU	2.3
1	A	613	ALA	2.3
1	A	347	SER	2.3
1	A	340	ARG	2.3
1	B	283	TYR	2.3
1	A	483	ASN	2.3
1	B	438	ASP	2.2
1	A	572	LEU	2.2
1	B	501	ALA	2.2
1	B	604	VAL	2.1
1	A	614	PRO	2.1
1	B	454	LEU	2.1
1	A	562	VAL	2.1
1	A	442	ASN	2.1
1	A	465	CYS	2.1
1	A	526	LEU	2.1
1	B	513	LEU	2.1
1	B	450	HIS	2.0
1	B	572	LEU	2.0
1	A	561	ILE	2.0
1	A	608	ILE	2.0

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	5XU	D	7	5/5	0.83	0.22	30,34,37,38	0
2	5XU	C	7	5/5	0.84	0.26	28,32,35,36	0
2	2KY	D	2	9/10	0.86	0.12	41,42,42,42	0
2	2KY	C	2	9/10	0.88	0.10	33,34,35,35	0
2	VEF	C	5	7/9	0.94	0.09	21,22,23,23	0
2	VEF	D	5	7/9	0.94	0.09	24,25,26,27	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
4	NAG	A	904	14/15	0.81	0.23	37,41,44,44	0
5	SO4	A	905	5/5	0.91	0.21	59,60,60,60	0
3	CA	A	903	1/1	0.96	0.08	30,30,30,30	0
3	CA	A	902	1/1	0.97	0.07	28,28,28,28	0
3	CA	B	901	1/1	0.98	0.06	24,24,24,24	0
3	CA	B	903	1/1	0.98	0.06	29,29,29,29	0
5	SO4	B	904	5/5	0.98	0.07	35,35,36,36	0
3	CA	A	901	1/1	0.99	0.06	22,22,22,22	0
3	CA	B	902	1/1	1.00	0.06	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.