



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:46 PM GMT

PDB ID : 4MOM
Title : Pyranose 2-oxidase H450G mutant with 3-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 1.90 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 ⓘ 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

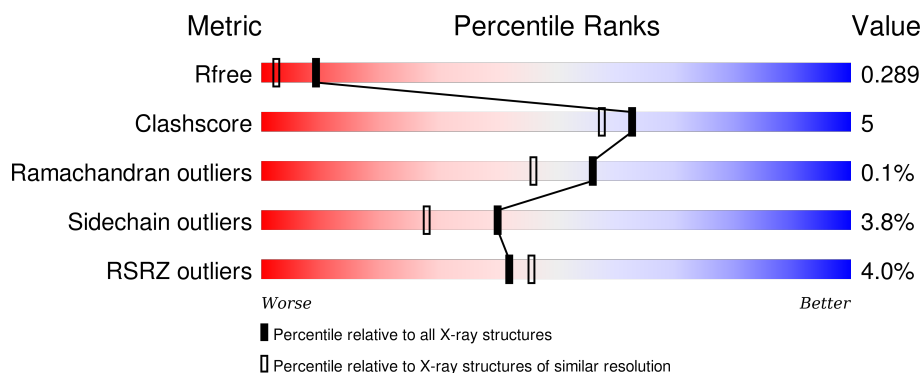
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	633	<div> <div>3%</div> <div>80% 11% 9%</div> </div>
1	B	633	<div> <div>2%</div> <div>78% 12% 9%</div> </div>
1	C	633	<div> <div>6%</div> <div>74% 16% 9%</div> </div>
1	D	633	<div> <div>3%</div> <div>77% 12% 9%</div> </div>

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
4	1PE	A	803	-	-	-	X
4	1PE	B	704	-	-	-	X
4	1PE	C	803	-	-	-	X
5	MES	B	701	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19522 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4536	2864	775	872	25			
1	B	576	Total	C	N	O	S	0	0	0
			4536	2864	775	872	25			
1	C	574	Total	C	N	O	S	0	0	0
			4520	2855	773	868	24			
1	D	574	Total	C	N	O	S	0	0	0
			4520	2855	773	868	24			

There are 52 discrepancies between the modelled and reference sequences:

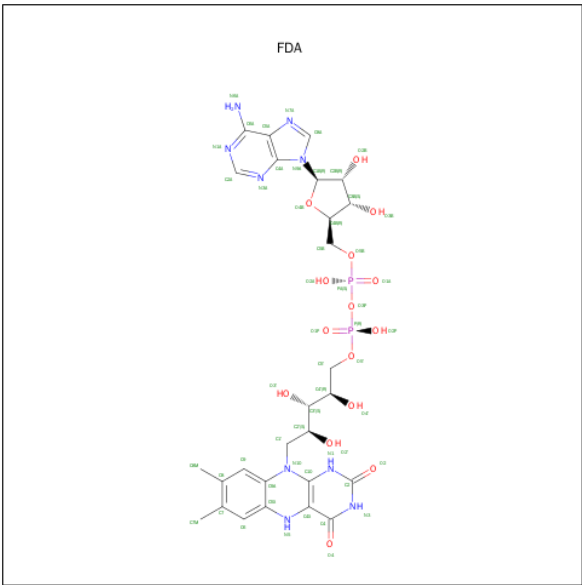
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
A	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
A	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
A	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
A	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
B	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
B	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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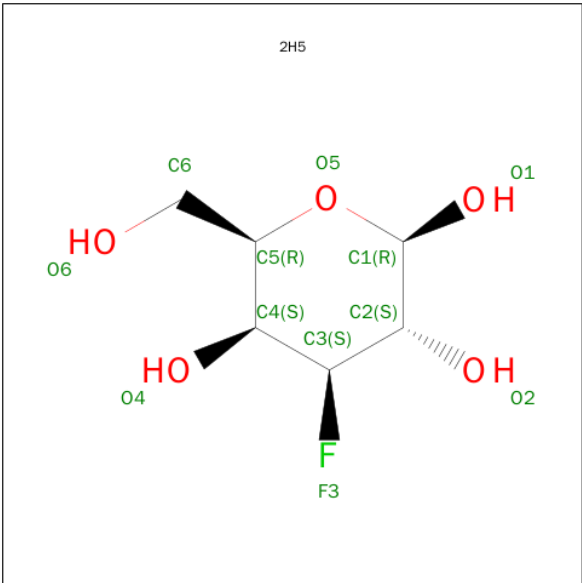
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
C	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
C	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
C	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
C	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	2	ALA	SER	CLONING ARTIFACT	UNP Q7ZA32
D	450	GLY	HIS	ENGINEERED MUTATION	UNP Q7ZA32
D	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
D	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
D	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



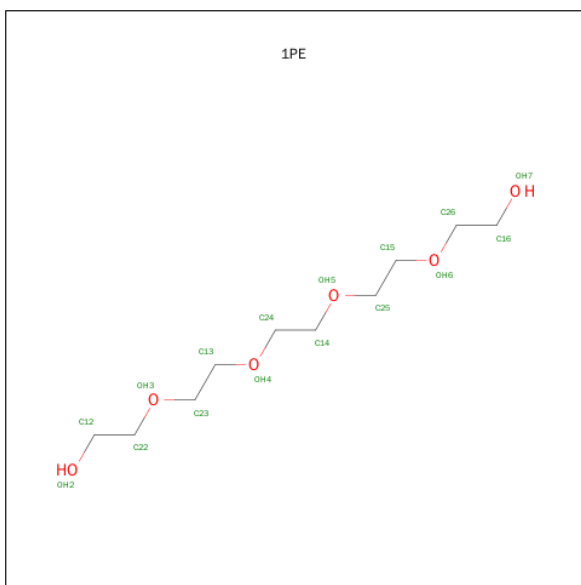
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 3-DEOXY-3-FLUORO-BETA-D-GALACTOPYRANOSE (three-letter code: 2H5) (formula: C₆H₁₁FO₅).



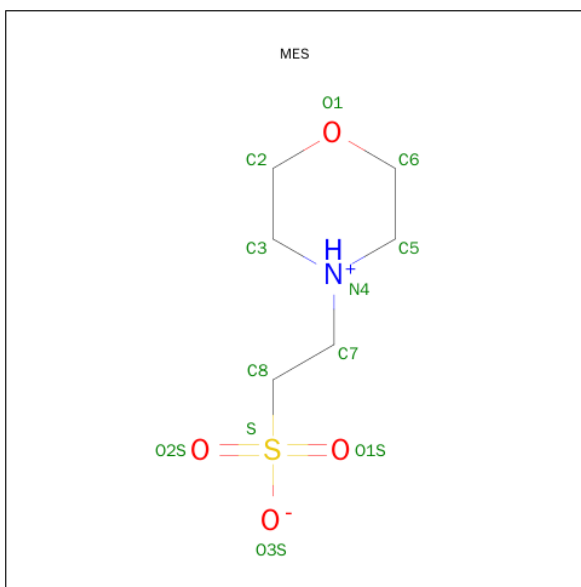
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 12	C 6	F 1	O 5	0	0
3	B	1	Total 12	C 6	F 1	O 5	0	0
3	C	1	Total 12	C 6	F 1	O 5	0	0
3	D	1	Total 12	C 6	F 1	O 5	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 12	C 8	O 4	0	0
4	B	1	Total 16	C 10	O 6	0	0
4	C	1	Total 16	C 10	O 6	0	0
4	D	1	Total 16	C 10	O 6	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			11	6	1	3	1		

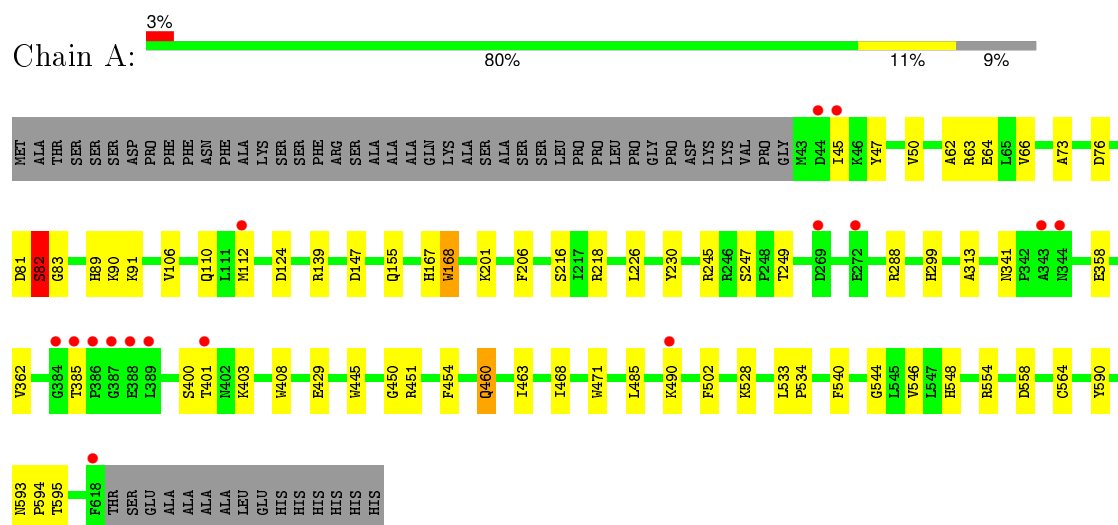
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total	O	0	0
			268	268		
6	B	348	Total	O	0	0
			348	348		
6	C	183	Total	O	0	0
			183	183		
6	D	268	Total	O	0	0
			268	268		

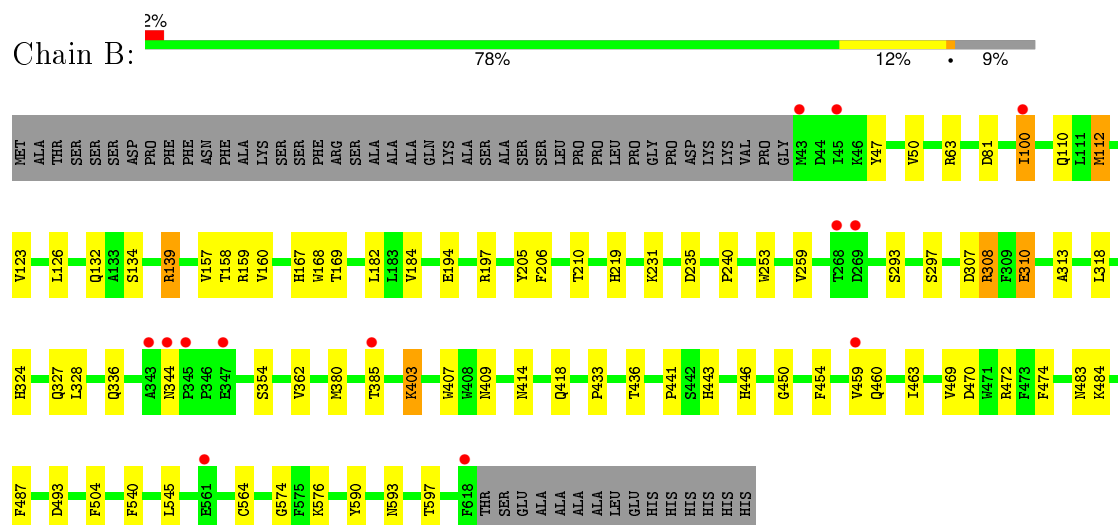
3 Residue-property plots [i](#)

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.

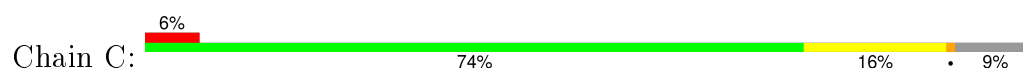
• Molecule 1: Pyranose 2-oxidase

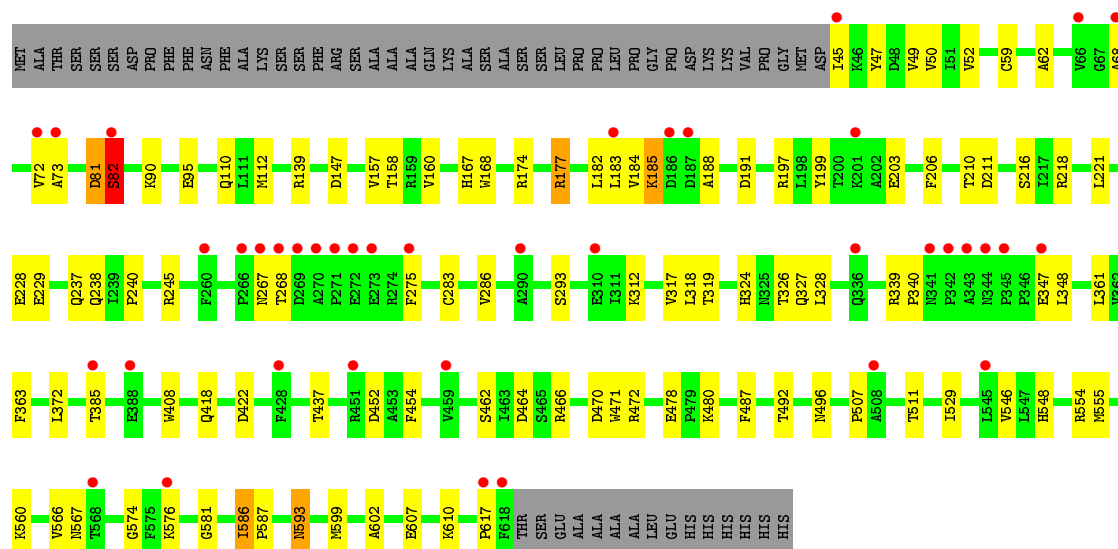


• Molecule 1: Pyranose 2-oxidase

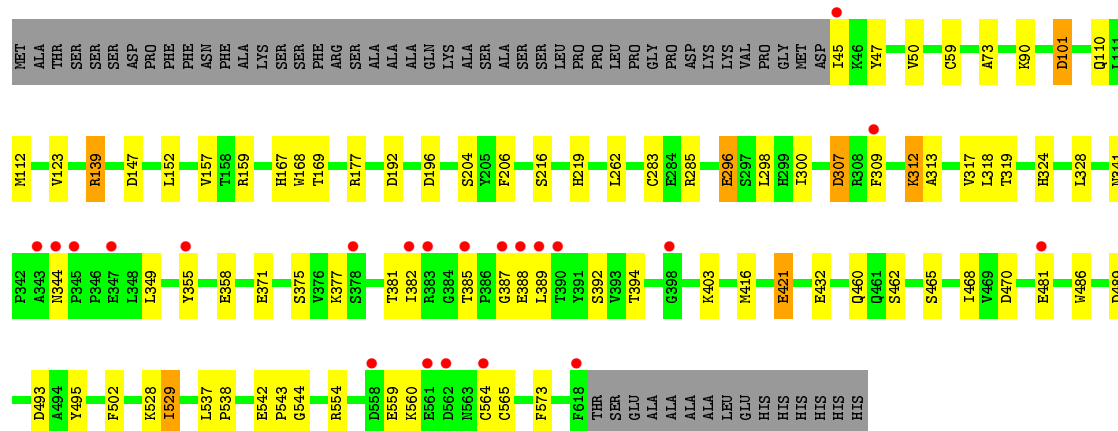
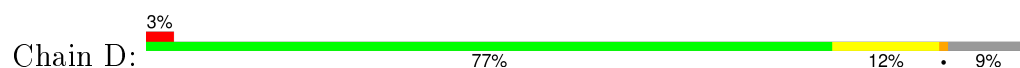


• Molecule 1: Pyranose 2-oxidase





• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.90Å 102.42Å 137.37Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 49.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-1.90) 99.2 (49.16-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.238 , 0.280 0.247 , 0.289	Depositor DCC
R_{free} test set	3865 reflections (1.82%)	DCC
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
Estimated twinning fraction	0.012 for -k,-h,-l 0.001 for k,h,-l 0.020 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 215838 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19522	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: FDA, 2H5, MES, 1PE

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	1.03	3/4651 (0.1%)	0.99	7/6323 (0.1%)
1	B	1.05	5/4651 (0.1%)	1.01	10/6323 (0.2%)
1	C	0.83	2/4635 (0.0%)	0.91	11/6302 (0.2%)
1	D	0.92	3/4635 (0.1%)	0.93	7/6302 (0.1%)
All	All	0.96	13/18572 (0.1%)	0.96	35/25250 (0.1%)

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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	CYS	CB-SG	-5.96	1.72	1.81
1	A	445	TRP	CD2-CE2	5.53	1.48	1.41
1	B	493	ASP	CB-CG	5.47	1.63	1.51
1	D	296	GLU	CD-OE1	5.42	1.31	1.25
1	B	407	TRP	CD2-CE2	5.41	1.47	1.41
1	D	486	TRP	CD2-CE2	5.23	1.47	1.41
1	B	253	TRP	CD2-CE2	5.22	1.47	1.41
1	D	147	ASP	CB-CG	5.19	1.62	1.51
1	A	168	TRP	CD2-CE2	5.14	1.47	1.41
1	A	471	TRP	CD2-CE2	5.13	1.47	1.41
1	C	408	TRP	CD2-CE2	5.12	1.47	1.41
1	B	597	THR	N-CA	-5.06	1.36	1.46
1	C	147	ASP	CB-CG	5.04	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	B	139	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	139	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	D	470	ASP	CB-CG-OD1	8.68	126.11	118.30
1	D	139	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	C	82	SER	N-CA-CB	7.72	122.09	110.50
1	B	493	ASP	CB-CG-OD1	6.85	124.47	118.30
1	D	139	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	211	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	283	CYS	CA-CB-SG	-6.32	102.62	114.00
1	A	147	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	63	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	D	493	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	139	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	466	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	245	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	422	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	B	308	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	288	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	245	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	174	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	308	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	81	ASP	N-CA-C	-5.67	95.70	111.00
1	C	464	ASP	CB-CG-OD1	5.57	123.32	118.30
1	C	81	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	C	245	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	81	ASP	CB-CG-OD1	-5.50	113.36	118.30
1	B	472	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	139	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	470	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	196	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	112	MET	CG-SD-CE	5.20	108.52	100.20
1	D	387	GLY	N-CA-C	5.14	125.94	113.10
1	B	307	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	235	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	436	THR	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	4536	0	4384	34	0
1	B	4536	0	4384	47	0
1	C	4520	0	4371	62	0
1	D	4520	0	4371	43	0
2	A	53	0	28	3	0
2	B	53	0	29	1	0
2	C	53	0	29	1	0
2	D	53	0	29	2	0
3	A	12	0	11	4	0
3	B	12	0	11	0	0
3	C	12	0	11	2	0
3	D	12	0	11	1	0
4	A	12	0	14	0	0
4	B	16	0	22	1	0
4	C	16	0	22	0	0
4	D	16	0	22	3	0
5	B	12	0	13	1	0
5	D	11	0	9	1	0
6	A	268	0	0	2	0
6	B	348	0	0	12	0
6	C	183	0	0	4	0
6	D	268	0	0	3	0
All	All	19522	0	17771	191	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 5.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:804:MES:C2	5:D:804:MES:C6	2.11	1.26
1:C:361:LEU:HD22	1:C:546:VAL:HG22	1.38	1.02
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.07	0.96
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.14	0.93
1:A:460:GLN:HE22	1:A:463:ILE:H	0.93	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ALA:HB2	1:C:610:LYS:HZ1	1.32	0.91
1:C:68:ALA:HB2	1:C:610:LYS:NZ	1.88	0.88
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.24	0.81
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.47	0.80
1:A:460:GLN:NE2	1:A:463:ILE:H	1.78	0.79
1:B:459:VAL:HG23	6:B:936:HOH:O	1.84	0.76
1:C:68:ALA:CB	1:C:610:LYS:NZ	2.49	0.75
1:B:418:GLN:HG3	6:B:1064:HOH:O	1.88	0.73
1:B:100:ILE:O	1:B:100:ILE:HD13	1.89	0.73
1:C:507:PRO:HD2	1:C:511:THR:HG21	1.72	0.72
1:D:421:GLU:N	1:D:421:GLU:OE1	2.20	0.71
1:D:432:GLU:N	1:D:432:GLU:OE1	2.24	0.70
1:C:68:ALA:CB	1:C:610:LYS:HZ3	2.04	0.69
1:C:81:ASP:OD1	1:C:81:ASP:C	2.29	0.68
1:C:218:ARG:HD2	6:C:1033:HOH:O	1.94	0.68
1:B:574:GLY:O	1:B:576:LYS:NZ	2.27	0.67
1:B:126:LEU:HD12	1:B:132:GLN:CG	2.25	0.66
2:C:801:FDA:N5	3:C:802:2H5:H1	2.11	0.66
1:C:361:LEU:CD2	1:C:546:VAL:HG22	2.19	0.65
1:A:460:GLN:HE22	1:A:463:ILE:N	1.79	0.64
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.30	0.64
1:C:177:ARG:HH22	1:C:188:ALA:HB1	1.63	0.64
1:B:328:LEU:C	1:B:328:LEU:HD23	2.17	0.64
1:D:169:THR:HG22	1:D:169:THR:O	1.98	0.63
1:D:489:ASP:C	1:D:489:ASP:OD1	2.37	0.63
4:D:803:1PE:H251	4:D:803:1PE:OH7	1.99	0.62
1:A:81:ASP:OD1	1:A:82:SER:N	2.31	0.61
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.48	0.61
1:B:545:LEU:HD12	6:B:1077:HOH:O	2.01	0.61
1:B:194:GLU:OE2	1:B:197:ARG:NH2	2.32	0.61
2:D:801:FDA:N5	3:D:802:2H5:H1	2.17	0.60
1:D:123:VAL:HG13	6:D:1110:HOH:O	2.01	0.60
1:D:157:VAL:HG11	1:D:324:HIS:CE1	2.37	0.60
4:D:803:1PE:C16	4:D:803:1PE:H251	2.30	0.59
1:B:336:GLN:NE2	1:B:344:ASN:O	2.35	0.59
1:D:318:LEU:HD13	1:D:328:LEU:HD22	1.84	0.59
1:C:81:ASP:OD1	1:C:82:SER:N	2.36	0.59
1:B:443:HIS:NE2	6:B:1013:HOH:O	2.32	0.58
4:B:704:1PE:H152	6:B:1094:HOH:O	2.03	0.57
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.38	0.57
1:A:230:TYR:OH	1:A:528:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:HIS:CE1	1:C:593:ASN:HA	2.41	0.55
1:C:318:LEU:HD13	1:C:328:LEU:HD23	1.87	0.55
1:B:126:LEU:HD12	1:B:132:GLN:HG3	1.89	0.55
1:C:199:TYR:O	1:C:203:GLU:HG3	2.07	0.55
1:B:403:LYS:HD2	6:B:1023:HOH:O	2.08	0.55
1:C:177:ARG:NH2	1:C:188:ALA:HB1	2.21	0.54
1:D:381:THR:HB	1:D:394:THR:OG1	2.08	0.54
1:C:317:VAL:HG12	1:C:319:THR:HG23	1.88	0.54
1:C:548:HIS:HE2	3:C:802:2H5:H9	1.55	0.54
1:C:237:GLN:NE2	1:C:238:GLN:O	2.37	0.54
1:B:414:ASN:O	1:B:418:GLN:HG2	2.08	0.54
1:C:228:GLU:OE1	1:C:229:GLU:OE2	2.25	0.54
1:A:124:ASP:O	1:D:543:PRO:HD3	2.08	0.54
1:D:47:TYR:CE2	1:D:73:ALA:HB2	2.43	0.53
1:B:297:SER:HB2	1:B:310:GLU:HG3	1.91	0.53
1:C:49:VAL:HB	1:C:72:VAL:HG22	1.91	0.53
1:D:375:SER:HA	6:D:1101:HOH:O	2.09	0.52
1:D:90:LYS:NZ	1:D:110:GLN:OE1	2.43	0.52
1:A:230:TYR:CZ	1:A:528:LYS:NZ	2.77	0.52
1:C:110:GLN:NE2	1:C:167:HIS:HD1	1.97	0.51
1:D:177:ARG:NH2	1:D:192:ASP:OD2	2.41	0.51
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.92	0.51
1:A:533:LEU:HD12	1:A:534:PRO:HD2	1.92	0.51
1:D:537:LEU:HB3	1:D:538:PRO:HD2	1.93	0.51
1:A:358:GLU:HG2	1:A:544:GLY:HA2	1.92	0.51
1:C:555:MET:HB2	1:C:566:VAL:HG23	1.92	0.51
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.41	0.50
1:A:548:HIS:NE2	3:A:802:2H5:O2	2.36	0.50
1:B:318:LEU:HD13	1:B:328:LEU:HD22	1.92	0.50
1:B:590:TYR:CZ	6:B:1002:HOH:O	2.55	0.50
1:C:361:LEU:HB2	1:C:546:VAL:HG21	1.94	0.50
1:A:554:ARG:O	1:A:564:CYS:HB2	2.11	0.50
1:B:483:ASN:OD1	1:B:504:PHE:HA	2.13	0.49
1:C:182:LEU:HD13	1:C:185:LYS:HA	1.95	0.49
1:C:183:LEU:O	1:C:184:VAL:HG23	2.13	0.49
1:A:546:VAL:HG22	1:A:546:VAL:O	2.12	0.48
1:A:249:THR:HG21	1:A:429:GLU:OE2	2.13	0.48
1:C:95:GLU:OE1	1:D:495:TYR:OH	2.21	0.48
1:D:371:GLU:CD	6:D:1039:HOH:O	2.52	0.48
1:D:528:LYS:C	1:D:529:ILE:HD13	2.34	0.47
1:C:206:PHE:CZ	1:C:599:MET:HE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:LEU:HD13	1:D:565:CYS:HB3	1.95	0.47
1:C:418:GLN:NE2	6:C:1051:HOH:O	2.37	0.47
1:A:362:VAL:HG12	1:A:540:PHE:CD1	2.49	0.47
1:B:354:SER:OG	1:B:484:LYS:NZ	2.46	0.47
1:A:47:TYR:CE2	1:A:73:ALA:HB2	2.50	0.47
1:C:347:GLU:HG3	1:C:348:LEU:HG	1.95	0.47
1:C:52:VAL:HG22	1:C:283:CYS:SG	2.54	0.47
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.96	0.47
1:D:317:VAL:HG12	1:D:319:THR:HG23	1.97	0.47
1:C:221:LEU:HD11	1:C:372:LEU:HD22	1.96	0.47
1:C:326:THR:HG22	1:C:487:PHE:HE2	1.80	0.46
1:D:216:SER:HB3	1:D:219:HIS:HB3	1.96	0.46
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.51	0.46
1:C:158:THR:HG22	1:C:160:VAL:HG22	1.97	0.46
1:D:157:VAL:HG11	1:D:324:HIS:HE1	1.80	0.46
1:D:47:TYR:CD2	1:D:73:ALA:HB2	2.50	0.46
1:D:529:ILE:HD13	1:D:529:ILE:N	2.30	0.46
1:C:555:MET:HE2	1:C:567:ASN:O	2.16	0.46
1:D:559:GLU:HG3	1:D:573:PHE:CD2	2.50	0.46
1:B:210:THR:HG23	6:B:1030:HOH:O	2.15	0.45
1:C:361:LEU:HB2	1:C:546:VAL:CG2	2.45	0.45
2:A:801:FDA:N5	3:A:802:2H5:H1	2.31	0.45
1:B:47:TYR:O	1:B:313:ALA:HA	2.15	0.45
1:A:548:HIS:CE1	3:A:802:2H5:O2	2.70	0.45
1:B:63:ARG:HD2	1:B:259:VAL:O	2.17	0.45
1:D:382:ILE:HD13	1:D:416:MET:HE1	1.97	0.45
1:C:327:GLN:HB2	1:C:487:PHE:CE1	2.52	0.45
1:B:293:SER:O	1:B:576:LYS:HG2	2.16	0.45
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.98	0.45
1:D:554:ARG:O	1:D:564:CYS:HB2	2.17	0.45
1:D:300:ILE:HD11	1:D:309:PHE:HB2	1.99	0.45
1:B:380:MET:HE3	1:B:409:ASN:OD1	2.16	0.45
1:A:548:HIS:CE1	3:A:802:2H5:H9	2.31	0.44
1:A:590:TYR:CD1	1:A:590:TYR:N	2.85	0.44
1:C:452:ASP:HB2	1:C:472:ARG:NH1	2.32	0.44
1:A:450:GLY:C	1:A:451:ARG:HG2	2.38	0.44
1:C:319:THR:HG22	1:C:581:GLY:HA3	1.99	0.44
1:B:446:HIS:HB3	1:B:474:PHE:HB2	1.99	0.44
1:A:47:TYR:O	1:A:313:ALA:HA	2.18	0.44
1:D:382:ILE:HD13	1:D:416:MET:CE	2.48	0.44
1:B:219:HIS:HA	1:B:433:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:VAL:O	1:C:286:VAL:HG23	2.18	0.44
1:A:62:ALA:O	1:A:66:VAL:HG23	2.18	0.43
1:D:296:GLU:O	1:D:312:LYS:NZ	2.34	0.43
1:C:197:ARG:NE	6:C:1019:HOH:O	2.45	0.43
1:D:169:THR:CG2	1:D:169:THR:O	2.64	0.43
1:C:158:THR:CG2	1:C:160:VAL:HG22	2.48	0.43
1:A:218:ARG:HD2	6:A:1045:HOH:O	2.17	0.43
1:B:327:GLN:HB2	1:B:487:PHE:CE1	2.53	0.43
1:B:450:GLY:O	1:B:470:ASP:HB2	2.18	0.43
1:B:469:VAL:HG23	6:B:939:HOH:O	2.17	0.43
1:C:363:PHE:HA	1:C:471:TRP:O	2.19	0.43
1:D:101:ASP:OD1	1:D:101:ASP:N	2.49	0.43
1:C:267:ASN:O	1:C:268:THR:C	2.55	0.43
1:B:126:LEU:HD12	1:B:132:GLN:HG2	1.98	0.43
1:D:465:SER:HA	1:D:468:ILE:HD12	2.01	0.43
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.43
1:D:307:ASP:N	1:D:307:ASP:OD1	2.51	0.42
1:C:293:SER:HA	1:C:574:GLY:O	2.19	0.42
1:C:59:CYS:HA	1:C:62:ALA:HB3	2.00	0.42
1:A:451:ARG:HD3	1:A:468:ILE:O	2.19	0.42
1:C:437:THR:HG23	1:C:437:THR:O	2.20	0.42
1:C:478:GLU:OE2	1:C:480:LYS:HE2	2.20	0.42
1:D:285:ARG:O	1:D:298:LEU:HD12	2.20	0.42
1:B:308:ARG:NH2	6:B:1024:HOH:O	2.53	0.42
1:C:586:ILE:HA	1:C:587:PRO:HD3	1.69	0.42
1:D:355:TYR:CZ	1:D:481:GLU:HB2	2.54	0.42
1:B:380:MET:HE1	1:B:409:ASN:HB3	2.01	0.42
1:A:590:TYR:CE2	1:A:594:PRO:HB3	2.55	0.42
1:A:81:ASP:O	1:A:83:GLY:N	2.46	0.42
1:C:206:PHE:CE2	1:C:599:MET:SD	3.13	0.42
1:C:72:VAL:O	1:C:275:PHE:HA	2.20	0.41
1:D:159:ARG:HA	2:D:801:FDA:O2B	2.21	0.41
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.94	0.41
1:B:403:LYS:CD	6:B:1023:HOH:O	2.66	0.41
1:D:389:LEU:HD23	1:D:389:LEU:HA	1.79	0.41
1:D:59:CYS:SG	1:D:262:LEU:HD21	2.61	0.41
1:B:182:LEU:HD22	1:B:184:VAL:O	2.20	0.41
1:B:362:VAL:HG12	1:B:540:PHE:CD1	2.55	0.41
1:B:158:THR:HG22	1:B:160:VAL:HG22	2.01	0.41
1:A:595:THR:OG1	2:A:801:FDA:O2	2.37	0.41
1:C:599:MET:O	1:C:602:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:THR:O	1:B:169:THR:HG22	2.19	0.41
1:B:63:ARG:NE	1:B:205:TYR:CE1	2.89	0.41
1:C:462:SER:O	1:D:139:ARG:HD2	2.21	0.41
1:D:152:LEU:HD12	1:D:502:PHE:CE1	2.56	0.41
4:D:803:IPE:C16	4:D:803:IPE:C25	2.96	0.40
1:A:155:GLN:NE2	1:A:358:GLU:OE2	2.52	0.40
1:B:219:HIS:HB2	1:B:433:PRO:HA	2.04	0.40
1:C:197:ARG:NH2	1:C:607:GLU:OE2	2.54	0.40
1:A:90:LYS:HD2	1:A:106:VAL:CG1	2.51	0.40
1:B:474:PHE:CD1	1:B:474:PHE:N	2.89	0.40
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.96	0.40
1:A:89:HIS:CE1	1:A:91:LYS:HB2	2.56	0.40
6:A:949:HOH:O	1:B:123:VAL:HG21	2.21	0.40
1:B:159:ARG:HA	2:B:702:FDA:O2B	2.22	0.40
1:B:132:GLN:NE2	5:B:701:MES:O1S	2.50	0.40
1:C:197:ARG:NH2	6:C:1019:HOH:O	2.51	0.40
1:A:485:LEU:HD13	1:A:502:PHE:CE1	2.56	0.40
1:B:460:GLN:OE1	1:B:463:ILE:N	2.35	0.40
1:B:418:GLN:CG	6:B:1064:HOH:O	2.60	0.40
1:A:76:ASP:OD1	2:A:801:FDA:O2B	2.28	0.40
1:C:372:LEU:HD11	1:C:529:ILE:HD12	2.03	0.40
1:D:358:GLU:HG2	1:D:544:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	574/633 (91%)	554 (96%)	19 (3%)	1 (0%)	52	42
1	B	574/633 (91%)	555 (97%)	19 (3%)	0	100	100
1	C	572/633 (90%)	547 (96%)	24 (4%)	1 (0%)	52	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	572/633 (90%)	547 (96%)	25 (4%)	0	100	100
All	All	2292/2532 (90%)	2203 (96%)	87 (4%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	C	617	PRO

5.3.2 Protein sidechains ⓘ

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	503/547 (92%)	482 (96%)	21 (4%)	36	24
1	B	503/547 (92%)	489 (97%)	14 (3%)	51	41
1	C	501/547 (92%)	480 (96%)	21 (4%)	36	24
1	D	501/547 (92%)	480 (96%)	21 (4%)	36	24
All	All	2008/2188 (92%)	1931 (96%)	77 (4%)	40	28

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	64	GLU
1	A	82	SER
1	A	112	MET
1	A	168	TRP
1	A	201	LYS
1	A	206	PHE
1	A	216	SER
1	A	247	SER
1	A	299	HIS
1	A	341	ASN
1	A	385	THR

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Mol	Chain	Res	Type
1	A	400	SER
1	A	401	THR
1	A	403	LYS
1	A	408	TRP
1	A	454	PHE
1	A	460	GLN
1	A	490	LYS
1	A	558	ASP
1	A	593	ASN
1	B	100	ILE
1	B	112	MET
1	B	134	SER
1	B	139	ARG
1	B	168	TRP
1	B	206	PHE
1	B	231	LYS
1	B	240	PRO
1	B	310	GLU
1	B	385	THR
1	B	403	LYS
1	B	441	PRO
1	B	454	PHE
1	B	593	ASN
1	C	45	ILE
1	C	50	VAL
1	C	82	SER
1	C	112	MET
1	C	168	TRP
1	C	177	ARG
1	C	185	LYS
1	C	191	ASP
1	C	210	THR
1	C	216	SER
1	C	240	PRO
1	C	312	LYS
1	C	385	THR
1	C	454	PHE
1	C	492	THR
1	C	496	ASN
1	C	554	ARG
1	C	560	LYS
1	C	576	LYS

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Mol	Chain	Res	Type
1	C	586	ILE
1	C	593	ASN
1	D	45	ILE
1	D	101	ASP
1	D	112	MET
1	D	168	TRP
1	D	204	SER
1	D	206	PHE
1	D	307	ASP
1	D	312	LYS
1	D	341	ASN
1	D	344	ASN
1	D	377	LYS
1	D	385	THR
1	D	388	GLU
1	D	392	SER
1	D	403	LYS
1	D	421	GLU
1	D	460	GLN
1	D	462	SER
1	D	529	ILE
1	D	542	GLU
1	D	560	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	341	ASN
1	A	460	GLN
1	B	110	GLN
1	B	344	ASN
1	B	611	GLN
1	C	110	GLN
1	C	207	GLN
1	C	263	GLN
1	C	461	GLN
1	D	132	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	418	GLN

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Mol	Chain	Res	Type
1	D	419	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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	FDA	A	801	1	48,58,58	1.46	6 (12%)	54,89,89	3.93	22 (40%)
3	2H5	A	802	-	12,12,12	1.32	1 (8%)	15,17,17	1.95	3 (20%)
4	1PE	A	803	-	11,11,15	0.68	0	10,10,14	0.28	0
5	MES	B	701	-	11,12,12	0.78	0	14,16,16	1.34	2 (14%)
2	FDA	B	702	1	48,58,58	1.59	11 (22%)	54,89,89	4.16	18 (33%)
3	2H5	B	703	-	12,12,12	1.08	0	15,17,17	2.36	6 (40%)
4	1PE	B	704	-	15,15,15	0.64	0	14,14,14	0.29	0
2	FDA	C	801	1	48,58,58	1.48	8 (16%)	54,89,89	4.28	17 (31%)
3	2H5	C	802	-	12,12,12	0.90	1 (8%)	15,17,17	3.34	6 (40%)
4	1PE	C	803	-	15,15,15	0.51	0	14,14,14	0.23	0
2	FDA	D	801	1	48,58,58	1.31	5 (10%)	54,89,89	3.53	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2H5	D	802	-	12,12,12	0.72	0	15,17,17	2.01	3 (20%)
4	1PE	D	803	-	15,15,15	0.62	0	14,14,14	0.22	0
5	MES	D	804	-	9,10,12	0.64	0	11,13,16	2.17	3 (27%)

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	FDA	A	801	1	-	0/30/50/50	0/6/6/6
3	2H5	A	802	-	-	0/2/22/22	0/1/1/1
4	1PE	A	803	-	-	0/9/9/13	0/0/0/0
5	MES	B	701	-	-	0/6/14/14	0/1/1/1
2	FDA	B	702	1	-	0/30/50/50	0/6/6/6
3	2H5	B	703	-	-	0/2/22/22	0/1/1/1
4	1PE	B	704	-	-	0/13/13/13	0/0/0/0
2	FDA	C	801	1	-	0/30/50/50	0/6/6/6
3	2H5	C	802	-	-	0/2/22/22	0/1/1/1
4	1PE	C	803	-	-	0/13/13/13	0/0/0/0
2	FDA	D	801	1	-	0/30/50/50	0/6/6/6
3	2H5	D	802	-	-	0/2/22/22	0/1/1/1
4	1PE	D	803	-	-	0/13/13/13	0/0/0/0
5	MES	D	804	-	-	0/10/10/14	0/0/0/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FDA	O3B-C3B	-3.96	1.33	1.43
2	B	702	FDA	O3B-C3B	-3.71	1.34	1.43
2	B	702	FDA	O4B-C1B	-3.25	1.37	1.41
2	A	801	FDA	C2'-C3'	-2.90	1.47	1.53
2	A	801	FDA	C9A-C5X	-2.81	1.36	1.42
2	B	702	FDA	O4B-C4B	-2.73	1.38	1.45
2	C	801	FDA	O4B-C4B	-2.71	1.38	1.45
2	A	801	FDA	O4B-C1B	-2.65	1.37	1.41
2	D	801	FDA	C2B-C3B	-2.53	1.46	1.53
2	B	702	FDA	C10-N1	-2.31	1.31	1.35
2	A	801	FDA	O4B-C4B	-2.15	1.40	1.45
2	B	702	FDA	C4X-N5	-2.14	1.30	1.33
2	B	702	FDA	PA-O1A	-2.12	1.43	1.51
2	C	801	FDA	O3B-C3B	-2.06	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	FDA	O3'-C3'	-2.06	1.38	1.43
3	C	802	2H5	C3-C4	2.07	1.53	1.52
2	B	702	FDA	C5'-C4'	2.13	1.54	1.51
2	D	801	FDA	C4-N3	2.23	1.37	1.33
2	C	801	FDA	C4X-N5	2.49	1.37	1.33
2	B	702	FDA	C1'-N10	2.52	1.51	1.48
2	C	801	FDA	C6-C5X	2.68	1.45	1.41
2	D	801	FDA	C2A-N3A	2.75	1.37	1.32
2	C	801	FDA	C9A-N10	2.89	1.42	1.38
2	B	702	FDA	C5X-N5	2.92	1.40	1.35
2	A	801	FDA	C4-C4X	3.11	1.47	1.41
2	C	801	FDA	C2A-N1A	3.20	1.40	1.33
3	A	802	2H5	C3-C4	3.56	1.55	1.52
2	C	801	FDA	C2A-N3A	3.65	1.38	1.32
2	D	801	FDA	C4'-C3'	3.65	1.60	1.53
2	D	801	FDA	C4-C4X	3.97	1.49	1.41
2	B	702	FDA	C4-C4X	4.13	1.49	1.41
2	C	801	FDA	C4-C4X	4.54	1.50	1.41

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	C4-C4X-C10	-22.46	105.57	119.94
2	D	801	FDA	C4-C4X-C10	-13.71	111.17	119.94
2	B	702	FDA	C4-C4X-C10	-13.17	111.51	119.94
2	C	801	FDA	N3A-C2A-N1A	-11.97	119.73	128.89
2	B	702	FDA	N3A-C2A-N1A	-11.66	119.97	128.89
2	A	801	FDA	N3A-C2A-N1A	-11.51	120.08	128.89
2	D	801	FDA	N3A-C2A-N1A	-10.24	121.06	128.89
2	A	801	FDA	C4-C4X-C10	-10.19	113.42	119.94
2	A	801	FDA	C4X-C4-N3	-10.01	109.91	123.59
2	B	702	FDA	C4X-C4-N3	-8.59	111.85	123.59
2	C	801	FDA	C4X-C4-N3	-6.20	115.11	123.59
2	C	801	FDA	C1B-N9A-C4A	-5.75	118.27	126.94
3	A	802	2H5	F3-C3-C2	-5.19	104.84	108.52
2	D	801	FDA	C4A-C5A-N7A	-5.04	104.84	109.48
2	D	801	FDA	C4X-C4-N3	-4.84	116.97	123.59
3	B	703	2H5	F3-C3-C2	-4.78	105.14	108.52
2	D	801	FDA	C4X-C10-N10	-4.76	117.71	120.52
2	C	801	FDA	C4X-C10-N10	-4.68	117.76	120.52
3	C	802	2H5	F3-C3-C2	-4.25	105.51	108.52
2	A	801	FDA	C4X-C10-N10	-3.85	118.25	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	C4B-O4B-C1B	-3.60	105.77	109.72
3	C	802	2H5	O6-C6-C5	-3.50	99.76	111.33
2	B	702	FDA	C7-C6-C5X	-3.45	115.28	120.92
5	B	701	MES	O1S-S-C8	-3.11	104.25	106.91
2	D	801	FDA	N6A-C6A-N1A	-2.92	112.94	119.20
2	A	801	FDA	O3P-P-O5'	-2.82	95.44	102.94
2	A	801	FDA	C9-C8-C7	-2.80	114.70	120.04
2	B	702	FDA	C7M-C7-C6	-2.75	112.81	120.28
2	A	801	FDA	C6-C5X-C9A	-2.58	115.59	118.98
2	B	702	FDA	O5'-P-O1P	-2.44	100.14	109.62
2	C	801	FDA	C4B-O4B-C1B	-2.40	107.08	109.72
5	D	804	MES	O3S-S-O2S	-2.39	106.05	111.61
3	B	703	2H5	O1-C1-C2	-2.37	102.86	109.21
2	A	801	FDA	C4B-O4B-C1B	-2.31	107.18	109.72
2	B	702	FDA	C4-C4X-N5	-2.19	116.06	118.72
2	C	801	FDA	C9A-C5X-N5	-2.12	119.23	122.36
2	B	702	FDA	C4X-C10-N10	-2.06	119.31	120.52
2	D	801	FDA	O5'-P-O1P	-2.00	101.84	109.62
2	D	801	FDA	O2A-PA-O1A	2.04	123.59	112.53
2	C	801	FDA	O3B-C3B-C2B	2.05	118.49	111.83
2	B	702	FDA	C5X-C9A-N10	2.07	119.19	117.62
2	C	801	FDA	O3B-C3B-C4B	2.16	117.54	111.05
3	C	802	2H5	C6-C5-C4	2.16	118.36	113.02
2	C	801	FDA	O4B-C4B-C3B	2.18	109.53	105.15
2	A	801	FDA	O2P-P-O5'	2.18	119.47	108.46
3	C	802	2H5	C3-C2-C1	2.18	114.63	110.46
2	A	801	FDA	C2A-N1A-C6A	2.20	122.70	118.77
2	B	702	FDA	O3P-PA-O5B	2.29	109.02	102.94
2	C	801	FDA	C4X-N5-C5X	2.34	119.46	116.76
2	D	801	FDA	O4B-C4B-C3B	2.34	109.87	105.15
3	C	802	2H5	O5-C5-C4	2.37	114.12	109.68
3	D	802	2H5	O5-C5-C6	2.43	112.50	106.36
3	A	802	2H5	O2-C2-C3	2.48	113.47	109.05
3	B	703	2H5	O5-C1-C2	2.51	113.79	109.80
2	B	702	FDA	O4B-C4B-C5B	2.52	118.33	109.32
2	A	801	FDA	O4B-C4B-C5B	2.55	118.46	109.32
2	D	801	FDA	O4B-C1B-N9A	2.78	113.91	108.10
2	B	702	FDA	O3B-C3B-C4B	2.79	119.43	111.05
3	D	802	2H5	O4-C4-C3	2.79	114.04	109.05
2	A	801	FDA	O4B-C4B-C3B	2.84	110.86	105.15
5	B	701	MES	O2S-S-C8	2.89	109.37	106.91
2	A	801	FDA	P-O3P-PA	2.89	140.85	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FDA	C5B-C4B-C3B	2.90	126.70	115.21
2	A	801	FDA	C4X-N5-C5X	2.90	120.10	116.76
2	A	801	FDA	C5B-C4B-C3B	2.97	127.00	115.21
2	B	702	FDA	C5B-C4B-C3B	2.99	127.09	115.21
3	A	802	2H5	F3-C3-C4	3.03	110.68	108.52
2	A	801	FDA	O2B-C2B-C3B	3.07	121.80	111.83
2	D	801	FDA	C4-C4X-N5	3.16	122.55	118.72
3	B	703	2H5	C3-C2-C1	3.17	116.51	110.46
2	A	801	FDA	C1'-N10-C9A	3.23	122.49	118.86
2	A	801	FDA	C6-C5X-N5	3.56	123.54	118.96
2	C	801	FDA	C4-C4X-N5	3.75	123.28	118.72
2	B	702	FDA	O4B-C1B-N9A	3.79	116.03	108.10
2	D	801	FDA	C1'-N10-C9A	3.79	123.12	118.86
3	B	703	2H5	F3-C3-C4	3.81	111.23	108.52
2	D	801	FDA	C5B-C4B-C3B	3.95	130.90	115.21
2	D	801	FDA	C4X-N5-C5X	4.13	121.51	116.76
2	A	801	FDA	O4B-C1B-N9A	4.13	116.75	108.10
2	C	801	FDA	O2B-C2B-C3B	4.27	125.72	111.83
3	B	703	2H5	O5-C5-C4	4.29	117.73	109.68
5	D	804	MES	O2S-S-C8	4.39	110.65	106.91
2	C	801	FDA	C5X-C9A-N10	4.40	120.97	117.62
2	D	801	FDA	O3B-C3B-C4B	4.60	124.86	111.05
5	D	804	MES	O1S-S-C8	4.63	110.86	106.91
2	C	801	FDA	C1'-N10-C9A	4.93	124.39	118.86
2	A	801	FDA	O3P-PA-O5B	5.07	116.38	102.94
3	D	802	2H5	F3-C3-C4	5.34	112.31	108.52
2	B	702	FDA	O2B-C2B-C3B	5.44	129.51	111.83
2	B	702	FDA	C2B-C1B-N9A	7.38	125.57	114.29
2	D	801	FDA	C4-N3-C2	7.80	121.99	115.25
2	A	801	FDA	C2B-C1B-N9A	9.02	128.08	114.29
2	C	801	FDA	C2B-C1B-N9A	9.03	128.09	114.29
2	B	702	FDA	C1'-N10-C9A	9.48	129.51	118.86
2	D	801	FDA	C2B-C1B-N9A	9.55	128.88	114.29
3	C	802	2H5	F3-C3-C4	10.68	116.10	108.52
2	A	801	FDA	C4-N3-C2	14.87	128.10	115.25
2	B	702	FDA	C4-N3-C2	16.06	129.13	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FDA	3	0
3	A	802	2H5	4	0
5	B	701	MES	1	0
2	B	702	FDA	1	0
4	B	704	1PE	1	0
2	C	801	FDA	1	0
3	C	802	2H5	2	0
2	D	801	FDA	2	0
3	D	802	2H5	1	0
4	D	803	1PE	3	0
5	D	804	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	576/633 (90%)	0.30	16 (2%) 56 60	11, 19, 37, 62	0
1	B	576/633 (90%)	0.36	13 (2%) 64 67	10, 18, 35, 61	0
1	C	574/633 (90%)	0.62	40 (6%) 19 21	14, 29, 51, 88	0
1	D	574/633 (90%)	0.45	22 (3%) 44 48	12, 22, 43, 64	0
All	All	2300/2532 (90%)	0.43	91 (3%) 42 46	10, 22, 44, 88	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	618	PHE	6.6
1	D	343	ALA	5.9
1	D	382	ILE	5.9
1	C	343	ALA	5.7
1	C	618	PHE	5.6
1	C	270	ALA	5.5
1	D	389	LEU	5.1
1	D	345	PRO	4.9
1	D	385	THR	4.8
1	C	344	ASN	4.7
1	C	272	GLU	4.5
1	C	345	PRO	4.3
1	D	390	THR	4.3
1	D	618	PHE	4.3
1	B	345	PRO	4.2
1	A	344	ASN	3.8
1	A	388	GLU	3.7
1	D	388	GLU	3.6
1	C	269	ASP	3.5
1	B	45	ILE	3.4
1	A	384	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	3.3
1	C	186	ASP	3.3
1	C	266	PRO	3.3
1	C	385	THR	3.3
1	D	398	GLY	3.2
1	C	617	PRO	3.2
1	B	269	ASP	3.2
1	C	271	PRO	3.2
1	D	344	ASN	3.1
1	D	355	TYR	3.1
1	C	290	ALA	3.1
1	B	344	ASN	3.1
1	D	387	GLY	3.0
1	A	45	ILE	2.9
1	A	343	ALA	2.8
1	C	342	PRO	2.8
1	C	45	ILE	2.7
1	D	558	ASP	2.7
1	B	268	THR	2.7
1	B	343	ALA	2.7
1	A	389	LEU	2.7
1	D	347	GLU	2.6
1	C	260	PHE	2.6
1	A	401	THR	2.6
1	D	378	SER	2.6
1	D	564	CYS	2.5
1	C	459	VAL	2.5
1	C	273	GLU	2.5
1	B	100	ILE	2.5
1	D	562	ASP	2.5
1	C	82	SER	2.4
1	A	272	GLU	2.4
1	C	428	PHE	2.4
1	B	43	MET	2.4
1	A	387	GLY	2.4
1	C	267	ASN	2.4
1	C	347	GLU	2.3
1	B	385	THR	2.3
1	C	275	PHE	2.3
1	D	383	ARG	2.3
1	A	385	THR	2.3
1	A	44	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	72	VAL	2.3
1	C	201	LYS	2.3
1	C	268	THR	2.3
1	C	183	LEU	2.2
1	A	490	LYS	2.2
1	C	68	ALA	2.2
1	C	568	THR	2.2
1	B	561	GLU	2.2
1	A	386	PRO	2.2
1	C	576	LYS	2.2
1	D	481	GLU	2.2
1	C	66	VAL	2.2
1	A	618	PHE	2.2
1	C	508	ALA	2.1
1	A	269	ASP	2.1
1	B	459	VAL	2.1
1	C	310	GLU	2.1
1	C	545	LEU	2.1
1	A	112	MET	2.1
1	D	309	PHE	2.1
1	C	187	ASP	2.1
1	C	336	GLN	2.1
1	B	347	GLU	2.0
1	C	341	ASN	2.0
1	D	561	GLU	2.0
1	C	451	ARG	2.0
1	C	388	GLU	2.0
1	C	73	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, 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
5	MES	B	701	12/12	0.93	0.22	4.27	28,38,41,44	0
4	1PE	A	803	12/16	0.82	0.20	4.22	27,31,36,36	0
4	1PE	C	803	16/16	0.74	0.25	3.87	43,50,64,69	0
4	1PE	B	704	16/16	0.84	0.19	2.38	28,41,53,54	0
4	1PE	D	803	16/16	0.84	0.17	1.61	31,37,48,51	0
3	2H5	A	802	12/12	0.87	0.14	0.89	29,31,34,34	0
3	2H5	C	802	12/12	0.86	0.15	0.61	39,42,47,50	0
5	MES	D	804	11/12	0.89	0.13	-0.32	31,38,44,49	0
3	2H5	B	703	12/12	0.92	0.12	-0.49	24,26,28,29	0
3	2H5	D	802	12/12	0.90	0.12	-0.63	26,30,33,34	0
2	FDA	A	801	53/53	0.97	0.10	-0.72	7,9,12,16	0
2	FDA	C	801	53/53	0.95	0.11	-0.83	18,20,28,32	0
2	FDA	B	702	53/53	0.97	0.10	-0.95	6,9,15,20	0
2	FDA	D	801	53/53	0.97	0.09	-1.44	11,13,19,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.