



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FSE  
Title : crystal structure of beta-site app-cleaving enzyme 1 (bace-wt) complex with N-(N-(4-amino-3,5- dichlorobenzyl)carbamimidoyl)-3-(4-methoxyphenyl)-5-methyl-4-isothiazolecarboxamide  
Authors : Muckelbauer, J.K.  
Deposited on : 2012-06-27  
Resolution : 2.65 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](mailto: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.

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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

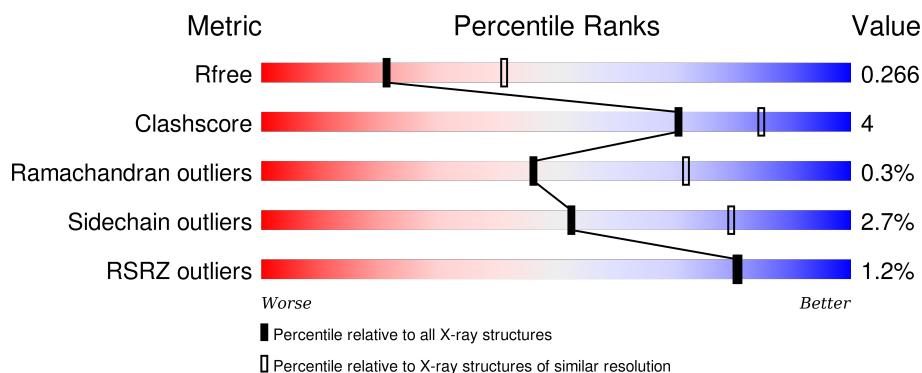
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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  $\geq 3$ , 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	455	<div> <div></div> <div>75% 9% • 15%</div> </div>
1	B	455	<div> <div></div> <div>75% 9% • 15%</div> </div>
1	D	455	<div> <div>2%</div> <div>75% 9% • 15%</div> </div>
1	E	455	<div> <div></div> <div>79% 5% • 15%</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
2	0VA	A	501	-	X	-	-
2	0VA	B	501	-	X	-	X
2	0VA	D	501	-	X	-	-
2	0VA	E	501	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12710 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3040	1946	505	575	14			
1	B	387	Total	C	N	O	S	0	0	0
			3032	1942	504	572	14			
1	D	387	Total	C	N	O	S	0	0	0
			3034	1942	505	573	14			
1	E	387	Total	C	N	O	S	0	0	0
			3040	1946	505	575	14			

There are 56 discrepancies between the modelled and reference sequences:

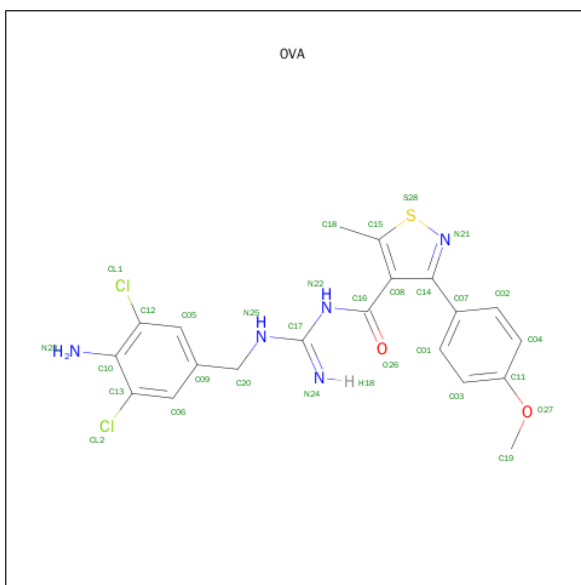
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP P56817
A	-12	ALA	-	EXPRESSION TAG	UNP P56817
A	-11	SER	-	EXPRESSION TAG	UNP P56817
A	-10	MET	-	EXPRESSION TAG	UNP P56817
A	-9	THR	-	EXPRESSION TAG	UNP P56817
A	-8	GLY	-	EXPRESSION TAG	UNP P56817
A	-7	GLY	-	EXPRESSION TAG	UNP P56817
A	-6	GLN	-	EXPRESSION TAG	UNP P56817
A	-5	GLN	-	EXPRESSION TAG	UNP P56817
A	-4	MET	-	EXPRESSION TAG	UNP P56817
A	-3	GLY	-	EXPRESSION TAG	UNP P56817
A	-2	ARG	-	EXPRESSION TAG	UNP P56817
A	-1	GLY	-	EXPRESSION TAG	UNP P56817
A	0	SER	-	EXPRESSION TAG	UNP P56817
B	-13	MET	-	EXPRESSION TAG	UNP P56817
B	-12	ALA	-	EXPRESSION TAG	UNP P56817
B	-11	SER	-	EXPRESSION TAG	UNP P56817
B	-10	MET	-	EXPRESSION TAG	UNP P56817
B	-9	THR	-	EXPRESSION TAG	UNP P56817
B	-8	GLY	-	EXPRESSION TAG	UNP P56817
B	-7	GLY	-	EXPRESSION TAG	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLN	-	EXPRESSION TAG	UNP P56817
B	-5	GLN	-	EXPRESSION TAG	UNP P56817
B	-4	MET	-	EXPRESSION TAG	UNP P56817
B	-3	GLY	-	EXPRESSION TAG	UNP P56817
B	-2	ARG	-	EXPRESSION TAG	UNP P56817
B	-1	GLY	-	EXPRESSION TAG	UNP P56817
B	0	SER	-	EXPRESSION TAG	UNP P56817
D	-13	MET	-	EXPRESSION TAG	UNP P56817
D	-12	ALA	-	EXPRESSION TAG	UNP P56817
D	-11	SER	-	EXPRESSION TAG	UNP P56817
D	-10	MET	-	EXPRESSION TAG	UNP P56817
D	-9	THR	-	EXPRESSION TAG	UNP P56817
D	-8	GLY	-	EXPRESSION TAG	UNP P56817
D	-7	GLY	-	EXPRESSION TAG	UNP P56817
D	-6	GLN	-	EXPRESSION TAG	UNP P56817
D	-5	GLN	-	EXPRESSION TAG	UNP P56817
D	-4	MET	-	EXPRESSION TAG	UNP P56817
D	-3	GLY	-	EXPRESSION TAG	UNP P56817
D	-2	ARG	-	EXPRESSION TAG	UNP P56817
D	-1	GLY	-	EXPRESSION TAG	UNP P56817
D	0	SER	-	EXPRESSION TAG	UNP P56817
E	-13	MET	-	EXPRESSION TAG	UNP P56817
E	-12	ALA	-	EXPRESSION TAG	UNP P56817
E	-11	SER	-	EXPRESSION TAG	UNP P56817
E	-10	MET	-	EXPRESSION TAG	UNP P56817
E	-9	THR	-	EXPRESSION TAG	UNP P56817
E	-8	GLY	-	EXPRESSION TAG	UNP P56817
E	-7	GLY	-	EXPRESSION TAG	UNP P56817
E	-6	GLN	-	EXPRESSION TAG	UNP P56817
E	-5	GLN	-	EXPRESSION TAG	UNP P56817
E	-4	MET	-	EXPRESSION TAG	UNP P56817
E	-3	GLY	-	EXPRESSION TAG	UNP P56817
E	-2	ARG	-	EXPRESSION TAG	UNP P56817
E	-1	GLY	-	EXPRESSION TAG	UNP P56817
E	0	SER	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is N-[N-(4-AMINO-3,5-DICHLOROBENZYL)CARBAMIMIDOYL]-3-(4-METHOXYPHENYL)-5-METHYL-1,2-THIAZOLE-4-CARBOXAMIDE (three-letter code: 0VA) (formula: C<sub>20</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 30	C 20	Cl 2	N 5	O 2	S 1	0	0
2	B	1	Total 30	C 20	Cl 2	N 5	O 2	S 1	0	0
2	D	1	Total 30	C 20	Cl 2	N 5	O 2	S 1	0	0
2	E	1	Total 30	C 20	Cl 2	N 5	O 2	S 1	0	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total 2 2	0	0
3	A	2	Total 2 2	0	0
3	D	2	Total 2 2	0	0
3	E	3	Total 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total 100 100	0	0

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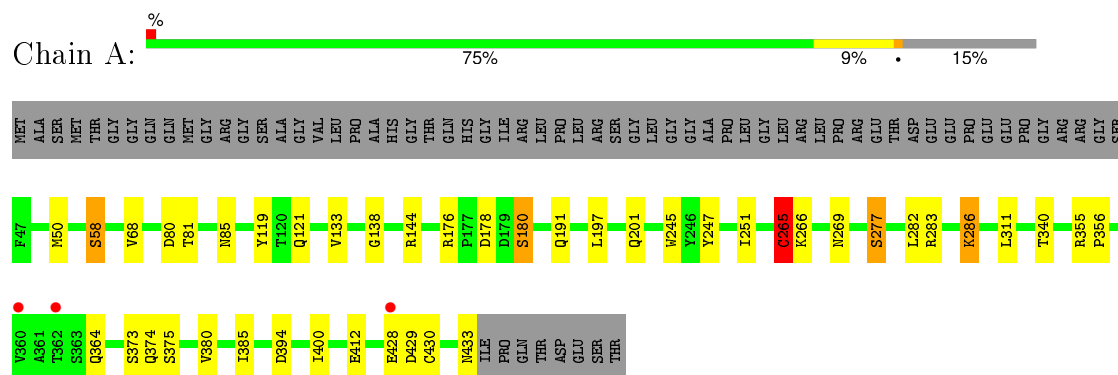
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	131	Total 131	O 131	0	0
4	D	106	Total 106	O 106	0	0
4	E	98	Total 98	O 98	0	0

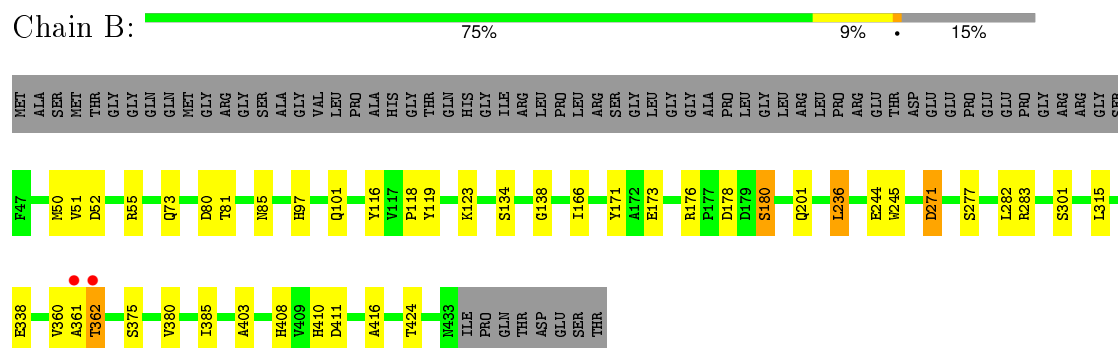
### 3 Residue-property plots

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.

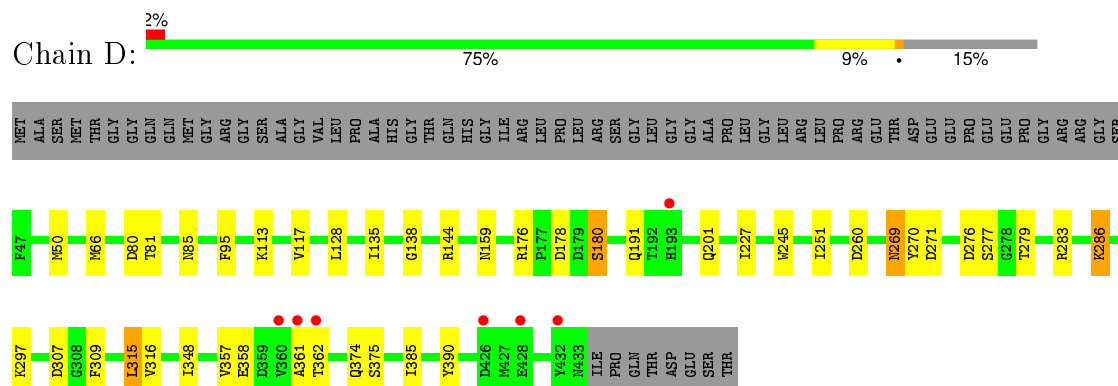
#### • Molecule 1: Beta-secretase 1



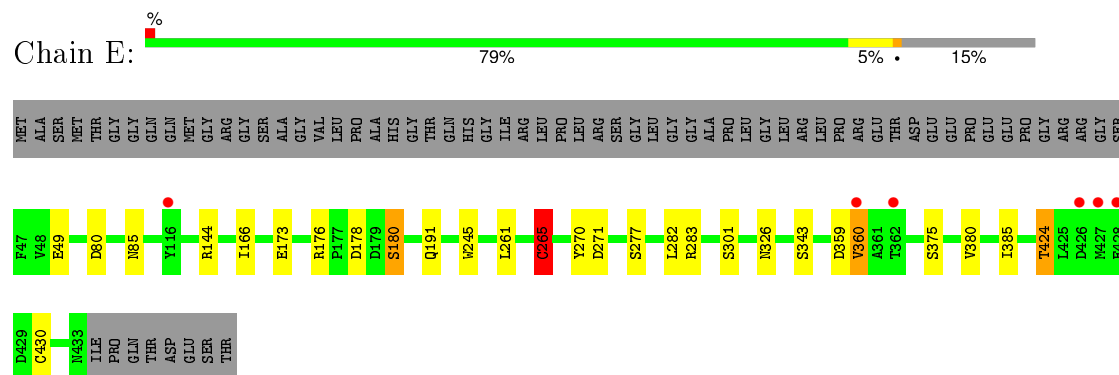
#### • Molecule 1: Beta-secretase 1



#### • Molecule 1: Beta-secretase 1



- Molecule 1: Beta-secretase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.33Å 131.22Å 88.95Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	44.08 – 2.65 44.08 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.08-2.65) 99.8 (44.08-2.65)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.217 , 0.267 0.217 , 0.266	Depositor DCC
$R_{free}$ test set	2891 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.6	EDS
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 56926 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8539e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 0VA, IOD

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	0.50	2/3118 (0.1%)	0.60	0/4240
1	B	0.47	0/3110	0.60	1/4230 (0.0%)
1	D	0.46	0/3112	0.60	0/4232
1	E	0.48	2/3118 (0.1%)	0.59	0/4240
All	All	0.48	4/12458 (0.0%)	0.60	1/16942 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	CYS	CB-SG	-8.04	1.68	1.82
1	A	430	CYS	CB-SG	-5.98	1.72	1.81
1	E	430	CYS	CB-SG	-5.85	1.72	1.81
1	E	265	CYS	CB-SG	-5.20	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ASP	N-CA-CB	-5.60	100.52	110.60

There are no chirality outliers.

There are no planarity outliers.

### 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	3040	0	2944	27	0
1	B	3032	0	2934	28	0
1	D	3034	0	2933	31	0
1	E	3040	0	2944	17	0
2	A	30	0	19	4	0
2	B	30	0	19	4	0
2	D	30	0	19	2	0
2	E	30	0	19	2	0
3	A	2	0	0	0	0
3	B	2	0	0	1	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
4	A	100	0	0	3	0
4	B	131	0	0	4	0
4	D	106	0	0	5	0
4	E	98	0	0	0	0
All	All	12710	0	11831	105	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 4.

All (105) 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:D:362:THR:HA	4:D:654:HOH:O	1.52	1.05
1:A:251:ILE:H	1:A:269:ASN:HD21	1.05	1.04
1:D:251:ILE:H	1:D:269:ASN:HD21	1.00	1.00
1:E:178:ASP:OD1	1:E:180:SER:HB2	1.62	0.99
1:B:55:ARG:HD3	4:B:700:HOH:O	1.69	0.90
1:D:358:GLU:HG3	4:D:654:HOH:O	1.70	0.90
2:A:501:OVA:N25	2:A:501:OVA:O26	2.06	0.89
1:B:73:GLN:HE22	1:B:101:GLN:H	1.21	0.89
1:A:85:ASN:HD21	1:A:176:ARG:H	1.23	0.87
1:D:178:ASP:OD1	1:D:180:SER:HB2	1.75	0.86
1:B:85:ASN:HD21	1:B:176:ARG:H	1.26	0.81
1:D:85:ASN:HD21	1:D:176:ARG:H	1.32	0.76
1:E:85:ASN:HD21	1:E:176:ARG:H	1.32	0.76
1:D:144:ARG:H	1:D:191:GLN:HE22	1.33	0.75
1:D:251:ILE:H	1:D:269:ASN:ND2	1.82	0.74
1:D:251:ILE:N	1:D:269:ASN:HD21	1.81	0.73
2:D:501:OVA:N25	2:D:501:OVA:O26	2.18	0.70
1:D:81:THR:H	1:D:277:SER:HB3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LYS:HD3	1:D:374:GLN:NE2	2.08	0.68
1:E:80:ASP:OD1	2:E:501:0VA:N24	2.27	0.67
1:D:361:ALA:HB3	4:D:704:HOH:O	1.93	0.67
1:A:251:ILE:H	1:A:269:ASN:ND2	1.88	0.66
1:E:144:ARG:H	1:E:191:GLN:HE22	1.42	0.65
1:D:348:ILE:HG12	4:D:687:HOH:O	1.96	0.65
1:D:178:ASP:OD1	1:D:180:SER:CB	2.46	0.64
1:A:429:ASP:HB2	4:A:675:HOH:O	1.97	0.64
1:D:309:PHE:CD1	1:D:316:VAL:HG23	2.33	0.64
1:A:282:LEU:HB2	1:A:385:ILE:HD11	1.80	0.64
2:E:501:0VA:O26	2:E:501:0VA:N25	2.29	0.62
1:A:178:ASP:OD1	1:A:180:SER:HB2	2.01	0.60
1:D:260:ASP:H	1:E:326:ASN:HD22	1.48	0.59
1:B:97:HIS:CD2	4:B:682:HOH:O	2.56	0.59
1:D:348:ILE:HD13	1:D:385:ILE:HD12	1.85	0.59
1:D:260:ASP:H	1:E:326:ASN:ND2	2.01	0.59
1:E:343:SER:HB3	1:E:424:THR:HG21	1.83	0.59
1:B:338:GLU:HG2	4:B:712:HOH:O	2.03	0.59
1:B:283:ARG:HB3	1:B:375:SER:HB2	1.85	0.58
1:D:283:ARG:HB3	1:D:375:SER:HB2	1.86	0.57
1:A:283:ARG:HB3	1:A:375:SER:HB2	1.87	0.57
1:B:80:ASP:OD1	2:B:501:0VA:N24	2.36	0.57
1:B:80:ASP:OD2	1:B:166:ILE:HD11	2.06	0.55
2:B:501:0VA:N25	2:B:501:0VA:O26	2.35	0.55
1:A:412:GLU:HG2	4:A:661:HOH:O	2.07	0.55
1:B:408:HIS:CE1	1:B:416:ALA:H	2.25	0.54
1:B:178:ASP:OD1	1:B:180:SER:HB2	2.07	0.54
1:E:283:ARG:HB3	1:E:375:SER:HB2	1.88	0.54
1:A:197:LEU:HD13	1:A:394:ASP:HA	1.90	0.53
1:B:201:GLN:HG3	1:B:201:GLN:O	2.09	0.52
1:D:201:GLN:HG3	1:D:201:GLN:O	2.10	0.52
1:D:80:ASP:OD1	2:D:501:0VA:N24	2.42	0.52
1:A:201:GLN:O	1:A:201:GLN:HG3	2.10	0.51
1:B:123:LYS:HG3	3:B:503:IOD:I	2.81	0.51
1:A:144:ARG:H	1:A:191:GLN:HE22	1.57	0.51
1:D:348:ILE:HD13	1:D:385:ILE:CD1	2.40	0.51
1:D:50:MET:HG2	1:D:138:GLY:HA2	1.92	0.51
1:D:144:ARG:HD3	4:D:670:HOH:O	2.09	0.51
1:E:178:ASP:OD1	1:E:180:SER:CB	2.48	0.50
1:B:361:ALA:HB3	4:B:702:HOH:O	2.10	0.50
1:E:343:SER:CB	1:E:424:THR:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:HIS:HD2	1:B:411:ASP:O	1.94	0.49
1:B:50:MET:HG2	1:B:138:GLY:HA2	1.94	0.49
1:B:362:THR:HG23	1:B:362:THR:O	2.12	0.48
1:A:80:ASP:OD1	2:A:501:0VA:N24	2.46	0.48
1:A:197:LEU:CD1	1:A:394:ASP:HA	2.43	0.48
1:E:343:SER:HB3	1:E:424:THR:CG2	2.44	0.47
1:A:50:MET:HG2	1:A:138:GLY:HA2	1.96	0.47
1:D:270:TYR:HA	1:D:271:ASP:HA	1.71	0.46
1:A:80:ASP:HA	1:A:277:SER:HB3	1.97	0.46
1:B:51:VAL:O	1:B:52:ASP:HB2	2.16	0.46
1:A:119:TYR:CD2	2:A:501:0VA:H5	2.51	0.45
1:D:117:VAL:HG22	1:D:176:ARG:HG3	1.99	0.45
1:A:283:ARG:HB2	1:A:380:VAL:HB	1.98	0.45
1:B:119:TYR:CD2	2:B:501:0VA:H5	2.52	0.45
1:B:80:ASP:CG	2:B:501:0VA:H18	2.20	0.45
1:E:282:LEU:HB2	1:E:385:ILE:HD11	1.99	0.45
1:B:171:TYR:CZ	1:B:244:GLU:HG2	2.51	0.45
1:E:359:ASP:OD1	1:E:360:VAL:N	2.49	0.45
1:B:178:ASP:OD1	1:B:180:SER:CB	2.65	0.45
1:B:282:LEU:HB2	1:B:385:ILE:HD11	1.99	0.45
1:B:81:THR:H	1:B:277:SER:HB3	1.82	0.44
1:E:270:TYR:HA	1:E:271:ASP:HA	1.85	0.44
1:A:247:TYR:HB3	1:A:400:ILE:HD11	2.00	0.44
1:A:81:THR:H	1:A:277:SER:HB2	1.83	0.43
1:E:80:ASP:OD2	1:E:166:ILE:HD11	2.17	0.43
1:D:315:LEU:HD23	1:D:357:VAL:HG21	1.99	0.43
1:E:283:ARG:HB2	1:E:380:VAL:HB	2.00	0.43
1:B:80:ASP:HA	1:B:277:SER:HB3	2.01	0.42
1:A:81:THR:H	1:A:277:SER:CB	2.33	0.42
1:A:144:ARG:N	1:A:191:GLN:HE22	2.17	0.42
1:D:113:LYS:CG	1:D:128:LEU:HD12	2.50	0.42
1:A:58:SER:HB2	4:A:614:HOH:O	2.20	0.42
1:B:236:LEU:HD13	1:B:403:ALA:HB2	2.01	0.41
1:A:266:LYS:HE3	1:A:429:ASP:O	2.20	0.41
1:A:355:ARG:HA	1:A:356:PRO:HD3	1.97	0.41
1:D:66:MET:HG2	1:D:135:ILE:HG12	2.03	0.41
1:B:283:ARG:HB2	1:B:380:VAL:HB	2.02	0.41
1:A:68:VAL:HG12	1:A:133:VAL:HG22	2.03	0.41
1:B:116:TYR:OH	1:B:118:PRO:HB3	2.20	0.41
1:E:261:LEU:HA	1:E:261:LEU:HD12	1.96	0.41
1:A:121:GLN:HG2	2:A:501:0VA:CL1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:HD3	1:A:374:GLN:NE2	2.36	0.41
1:D:276:ASP:OD2	1:D:279:THR:OG1	2.37	0.40
1:D:95:PHE:CE1	1:D:159:ASN:HB2	2.57	0.40
1:D:227:ILE:HG23	1:D:390:TYR:HE2	1.86	0.40
1:B:173:GLU:HG3	1:B:173:GLU:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/455 (85%)	373 (97%)	10 (3%)	2 (0%)	34	59
1	B	385/455 (85%)	374 (97%)	11 (3%)	0	100	100
1	D	385/455 (85%)	372 (97%)	12 (3%)	1 (0%)	46	72
1	E	385/455 (85%)	372 (97%)	12 (3%)	1 (0%)	46	72
All	All	1540/1820 (85%)	1491 (97%)	45 (3%)	4 (0%)	46	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	CYS
1	E	265	CYS
1	A	286	LYS
1	D	286	LYS

### 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	329/381 (86%)	318 (97%)	11 (3%)	45	73
1	B	327/381 (86%)	317 (97%)	10 (3%)	47	75
1	D	327/381 (86%)	321 (98%)	6 (2%)	66	88
1	E	329/381 (86%)	320 (97%)	9 (3%)	52	80
All	All	1312/1524 (86%)	1276 (97%)	36 (3%)	52	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	180	SER
1	A	245	TRP
1	A	265	CYS
1	A	277	SER
1	A	311	LEU
1	A	340	THR
1	A	364	GLN
1	A	373	SER
1	A	428	GLU
1	A	433	ASN
1	B	134	SER
1	B	180	SER
1	B	236	LEU
1	B	245	TRP
1	B	271	ASP
1	B	301	SER
1	B	315	LEU
1	B	360	VAL
1	B	362	THR
1	B	424	THR
1	D	180	SER
1	D	245	TRP
1	D	269	ASN
1	D	297	LYS
1	D	307	ASP
1	D	315	LEU
1	E	49	GLU
1	E	173	GLU
1	E	180	SER

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Mol	Chain	Res	Type
1	E	245	TRP
1	E	265	CYS
1	E	277	SER
1	E	301	SER
1	E	360	VAL
1	E	424	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	146	ASN
1	A	191	GLN
1	A	201	GLN
1	A	259	GLN
1	A	269	ASN
1	A	342	GLN
1	A	374	GLN
1	B	73	GLN
1	B	85	ASN
1	B	97	HIS
1	B	146	ASN
1	B	211	GLN
1	B	229	HIS
1	B	259	GLN
1	B	341	ASN
1	B	408	HIS
1	B	410	HIS
1	D	76	ASN
1	D	85	ASN
1	D	191	GLN
1	D	229	HIS
1	D	259	GLN
1	D	269	ASN
1	D	341	ASN
1	D	374	GLN
1	D	410	HIS
1	E	76	ASN
1	E	85	ASN
1	E	146	ASN
1	E	159	ASN
1	E	191	GLN

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Mol	Chain	Res	Type
1	E	229	HIS
1	E	259	GLN
1	E	326	ASN
1	E	341	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\# Z  > 2$
2	0VA	A	501	-	30,32,32	6.40	24 (80%)	34,45,45	4.83	21 (61%)
2	0VA	B	501	-	30,32,32	6.60	25 (83%)	34,45,45	4.61	22 (64%)
2	0VA	D	501	-	30,32,32	6.38	24 (80%)	34,45,45	4.63	22 (64%)
2	0VA	E	501	-	30,32,32	6.52	24 (80%)	34,45,45	4.76	19 (55%)

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	0VA	A	501	-	-	0/14/19/19	0/2/3/3
2	0VA	B	501	-	-	0/14/19/19	0/2/3/3
2	0VA	D	501	-	-	0/14/19/19	0/2/3/3
2	0VA	E	501	-	-	0/14/19/19	0/2/3/3

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	0VA	C12-CL1	2.56	1.79	1.73
2	E	501	0VA	O27-C11	2.72	1.43	1.37
2	A	501	0VA	O27-C11	2.72	1.43	1.37
2	B	501	0VA	C15-S28	2.85	1.76	1.71
2	D	501	0VA	O27-C11	2.90	1.44	1.37
2	A	501	0VA	C15-S28	2.96	1.76	1.71
2	B	501	0VA	O27-C11	3.00	1.44	1.37
2	D	501	0VA	C15-S28	3.40	1.77	1.71
2	D	501	0VA	C07-C14	3.46	1.52	1.49
2	A	501	0VA	C07-C14	3.55	1.52	1.49
2	E	501	0VA	C10-N23	3.87	1.48	1.37
2	E	501	0VA	C15-S28	3.92	1.78	1.71
2	B	501	0VA	C10-N23	4.01	1.49	1.37
2	A	501	0VA	C10-N23	4.02	1.49	1.37
2	D	501	0VA	C10-N23	4.09	1.49	1.37
2	B	501	0VA	C07-C14	4.21	1.53	1.49
2	E	501	0VA	C07-C14	4.40	1.53	1.49
2	D	501	0VA	C17-N22	4.94	1.46	1.37
2	A	501	0VA	C17-N22	5.15	1.46	1.37
2	E	501	0VA	C17-N25	5.18	1.46	1.34
2	E	501	0VA	C17-N22	5.19	1.46	1.37
2	B	501	0VA	C17-N22	5.28	1.46	1.37
2	A	501	0VA	C17-N25	5.29	1.46	1.34
2	D	501	0VA	C17-N25	5.51	1.47	1.34
2	B	501	0VA	C17-N25	5.57	1.47	1.34
2	D	501	0VA	C16-N22	6.56	1.49	1.37
2	D	501	0VA	C01-C07	6.60	1.53	1.39
2	A	501	0VA	C16-N22	6.72	1.49	1.37
2	E	501	0VA	C16-N22	6.73	1.49	1.37
2	B	501	0VA	C06-C09	6.74	1.51	1.39
2	D	501	0VA	C06-C09	6.83	1.51	1.39
2	A	501	0VA	C06-C09	6.86	1.51	1.39
2	B	501	0VA	C16-N22	7.00	1.50	1.37
2	A	501	0VA	C01-C07	7.05	1.54	1.39
2	B	501	0VA	C01-C07	7.09	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	0VA	C17-N24	7.13	1.47	1.29
2	E	501	0VA	C04-C11	7.17	1.53	1.38
2	E	501	0VA	C01-C07	7.19	1.54	1.39
2	A	501	0VA	C02-C07	7.21	1.54	1.39
2	D	501	0VA	C04-C11	7.22	1.53	1.38
2	E	501	0VA	C06-C09	7.24	1.52	1.39
2	D	501	0VA	C02-C07	7.24	1.54	1.39
2	D	501	0VA	C05-C09	7.25	1.52	1.39
2	A	501	0VA	C04-C11	7.29	1.53	1.38
2	B	501	0VA	C17-N24	7.32	1.47	1.29
2	E	501	0VA	C10-C13	7.34	1.52	1.40
2	E	501	0VA	C02-C07	7.35	1.55	1.39
2	A	501	0VA	C05-C09	7.35	1.52	1.39
2	D	501	0VA	C03-C11	7.37	1.53	1.38
2	A	501	0VA	C17-N24	7.40	1.48	1.29
2	B	501	0VA	C03-C11	7.40	1.53	1.38
2	D	501	0VA	C17-N24	7.45	1.48	1.29
2	B	501	0VA	C04-C11	7.46	1.53	1.38
2	E	501	0VA	C10-C12	7.49	1.52	1.40
2	A	501	0VA	C08-C15	7.50	1.51	1.38
2	E	501	0VA	C05-C09	7.52	1.52	1.39
2	A	501	0VA	C10-C13	7.54	1.52	1.40
2	E	501	0VA	C08-C15	7.62	1.51	1.38
2	B	501	0VA	C02-C07	7.63	1.55	1.39
2	D	501	0VA	C10-C12	7.67	1.52	1.40
2	E	501	0VA	C03-C11	7.75	1.54	1.38
2	D	501	0VA	C08-C15	7.81	1.51	1.38
2	B	501	0VA	C08-C15	7.81	1.51	1.38
2	A	501	0VA	C03-C11	7.82	1.54	1.38
2	D	501	0VA	C05-C12	7.84	1.51	1.38
2	B	501	0VA	C10-C13	7.91	1.53	1.40
2	D	501	0VA	C10-C13	7.92	1.53	1.40
2	B	501	0VA	C06-C13	7.93	1.51	1.38
2	A	501	0VA	C10-C12	7.98	1.53	1.40
2	E	501	0VA	C06-C13	8.00	1.52	1.38
2	B	501	0VA	C05-C09	8.01	1.53	1.39
2	A	501	0VA	C02-C04	8.01	1.53	1.38
2	B	501	0VA	C10-C12	8.03	1.53	1.40
2	D	501	0VA	C06-C13	8.08	1.52	1.38
2	A	501	0VA	C05-C12	8.12	1.52	1.38
2	A	501	0VA	C06-C13	8.15	1.52	1.38
2	E	501	0VA	C02-C04	8.19	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	0VA	C14-N21	8.31	1.48	1.33
2	E	501	0VA	C05-C12	8.32	1.52	1.38
2	B	501	0VA	C01-C03	8.33	1.53	1.38
2	D	501	0VA	C01-C03	8.42	1.53	1.38
2	D	501	0VA	C14-N21	8.46	1.48	1.33
2	D	501	0VA	C02-C04	8.48	1.54	1.38
2	B	501	0VA	C14-N21	8.55	1.48	1.33
2	A	501	0VA	C01-C03	8.56	1.54	1.38
2	E	501	0VA	C14-N21	8.79	1.49	1.33
2	B	501	0VA	C02-C04	8.81	1.54	1.38
2	E	501	0VA	C01-C03	8.90	1.54	1.38
2	B	501	0VA	C05-C12	9.10	1.53	1.38
2	D	501	0VA	O26-C16	9.76	1.43	1.23
2	A	501	0VA	O26-C16	9.76	1.43	1.23
2	D	501	0VA	C08-C14	9.78	1.52	1.41
2	A	501	0VA	C08-C14	9.82	1.52	1.41
2	B	501	0VA	C08-C14	9.94	1.52	1.41
2	E	501	0VA	C08-C14	10.11	1.52	1.41
2	B	501	0VA	O26-C16	10.29	1.44	1.23
2	E	501	0VA	O26-C16	10.42	1.44	1.23

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0VA	C08-C14-N21	-9.31	103.73	114.75
2	E	501	0VA	C08-C14-N21	-8.71	104.45	114.75
2	D	501	0VA	C08-C14-N21	-8.56	104.62	114.75
2	E	501	0VA	C02-C07-C14	-8.33	107.61	120.60
2	A	501	0VA	C08-C14-N21	-8.19	105.07	114.75
2	A	501	0VA	C02-C07-C14	-8.06	108.03	120.60
2	D	501	0VA	C02-C07-C14	-6.53	110.41	120.60
2	E	501	0VA	O26-C16-N22	-6.15	112.82	122.36
2	A	501	0VA	O26-C16-N22	-6.15	112.82	122.36
2	B	501	0VA	C02-C07-C14	-6.01	111.22	120.60
2	A	501	0VA	O26-C16-C08	-5.98	112.12	120.80
2	B	501	0VA	O26-C16-C08	-5.86	112.30	120.80
2	D	501	0VA	O26-C16-N22	-5.40	113.98	122.36
2	D	501	0VA	O26-C16-C08	-5.34	113.06	120.80
2	D	501	0VA	C20-C09-C05	-5.01	111.74	120.62
2	B	501	0VA	O26-C16-N22	-4.95	114.69	122.36
2	E	501	0VA	O26-C16-C08	-4.65	114.05	120.80
2	A	501	0VA	C20-C09-C05	-4.32	112.97	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	0VA	C20-C09-C05	-4.12	113.31	120.62
2	E	501	0VA	C02-C07-C01	-3.74	110.47	117.55
2	B	501	0VA	C02-C07-C01	-3.64	110.66	117.55
2	D	501	0VA	C02-C07-C01	-3.56	110.82	117.55
2	B	501	0VA	C20-C09-C05	-3.56	114.32	120.62
2	D	501	0VA	C04-C11-C03	-3.38	114.72	120.20
2	B	501	0VA	C04-C11-C03	-3.28	114.87	120.20
2	D	501	0VA	C13-C10-C12	-3.23	112.58	115.01
2	A	501	0VA	C02-C07-C01	-3.18	111.53	117.55
2	A	501	0VA	C20-N25-C17	-3.02	118.88	122.38
2	E	501	0VA	C04-C11-C03	-3.00	115.33	120.20
2	A	501	0VA	C13-C10-C12	-2.97	112.77	115.01
2	A	501	0VA	C04-C11-C03	-2.81	115.63	120.20
2	B	501	0VA	C05-C12-C10	-2.62	121.32	123.13
2	B	501	0VA	C13-C10-C12	-2.43	113.17	115.01
2	B	501	0VA	C06-C13-CL2	-2.38	114.83	118.50
2	D	501	0VA	C20-N25-C17	-2.07	119.98	122.38
2	E	501	0VA	C13-C10-C12	-2.03	113.48	115.01
2	B	501	0VA	O27-C11-C04	2.06	129.73	119.78
2	A	501	0VA	C01-C03-C11	2.07	122.36	119.74
2	D	501	0VA	C01-C03-C11	2.24	122.56	119.74
2	D	501	0VA	C10-C12-CL1	2.24	120.81	117.76
2	E	501	0VA	C03-C01-C07	2.37	124.60	121.14
2	B	501	0VA	C01-C03-C11	2.38	122.74	119.74
2	E	501	0VA	C09-C20-N25	2.45	118.47	112.88
2	D	501	0VA	C03-C01-C07	2.52	124.82	121.14
2	B	501	0VA	C03-C01-C07	2.52	124.83	121.14
2	D	501	0VA	C09-C20-N25	2.56	118.73	112.88
2	A	501	0VA	C19-O27-C11	2.67	123.76	117.51
2	A	501	0VA	C10-C12-CL1	2.70	121.44	117.76
2	E	501	0VA	C19-O27-C11	2.99	124.52	117.51
2	D	501	0VA	C12-C05-C09	3.01	122.31	120.36
2	E	501	0VA	C12-C05-C09	3.17	122.41	120.36
2	B	501	0VA	C04-C02-C07	3.27	125.91	121.14
2	A	501	0VA	C12-C05-C09	3.31	122.50	120.36
2	D	501	0VA	C04-C02-C07	3.34	126.02	121.14
2	A	501	0VA	C09-C20-N25	3.37	120.58	112.88
2	E	501	0VA	C06-C13-C10	3.45	125.51	123.13
2	A	501	0VA	C04-C02-C07	3.70	126.55	121.14
2	D	501	0VA	C19-O27-C11	3.75	126.30	117.51
2	E	501	0VA	C04-C02-C07	3.92	126.86	121.14
2	D	501	0VA	C06-C13-C10	4.02	125.90	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	0VA	C19-O27-C11	4.03	126.94	117.51
2	B	501	0VA	C12-C05-C09	4.35	123.18	120.36
2	A	501	0VA	C06-C13-C10	4.38	126.15	123.13
2	B	501	0VA	C20-C09-C06	4.85	129.21	120.62
2	B	501	0VA	C06-C13-C10	4.98	126.56	123.13
2	A	501	0VA	C20-C09-C06	5.40	130.18	120.62
2	E	501	0VA	C20-C09-C06	5.44	130.25	120.62
2	D	501	0VA	C20-C09-C06	6.00	131.25	120.62
2	A	501	0VA	C15-C08-C14	6.03	116.00	105.27
2	D	501	0VA	C15-C08-C14	6.14	116.19	105.27
2	E	501	0VA	C15-C08-C14	6.14	116.19	105.27
2	B	501	0VA	C15-C08-C14	6.64	117.08	105.27
2	A	501	0VA	C14-N21-S28	7.50	115.86	104.81
2	D	501	0VA	C14-N21-S28	7.97	116.56	104.81
2	B	501	0VA	C14-N21-S28	8.07	116.70	104.81
2	E	501	0VA	C14-N21-S28	8.20	116.89	104.81
2	B	501	0VA	C01-C07-C14	11.16	138.01	120.60
2	B	501	0VA	C08-C16-N22	11.21	132.65	114.76
2	D	501	0VA	C08-C16-N22	11.30	132.80	114.76
2	E	501	0VA	C08-C16-N22	11.33	132.85	114.76
2	D	501	0VA	C01-C07-C14	11.64	138.76	120.60
2	A	501	0VA	C08-C16-N22	12.57	134.82	114.76
2	A	501	0VA	C01-C07-C14	12.69	140.40	120.60
2	E	501	0VA	C01-C07-C14	13.60	141.83	120.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	0VA	4	0
2	B	501	0VA	4	0
2	D	501	0VA	2	0
2	E	501	0VA	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/455 (85%)	-0.30	3 (0%) 87 87	10, 20, 33, 39	0
1	B	387/455 (85%)	-0.29	2 (0%) 91 92	10, 20, 33, 39	0
1	D	387/455 (85%)	-0.15	7 (1%) 71 70	10, 20, 33, 39	0
1	E	387/455 (85%)	-0.28	6 (1%) 74 74	11, 20, 33, 40	0
All	All	1548/1820 (85%)	-0.26	18 (1%) 81 80	10, 20, 33, 40	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	THR	5.6
1	D	360	VAL	5.1
1	D	361	ALA	4.3
1	D	362	THR	3.4
1	A	360	VAL	3.2
1	E	362	THR	3.0
1	A	362	THR	2.9
1	D	193	HIS	2.7
1	E	360	VAL	2.6
1	A	428	GLU	2.6
1	E	428	GLU	2.5
1	D	432	TYR	2.4
1	E	116	TYR	2.4
1	B	361	ALA	2.4
1	D	426	ASP	2.3
1	E	426	ASP	2.1
1	E	427	MET	2.1
1	D	428	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	0VA	B	501	30/30	0.90	0.25	2.07	28,30,33,33	0
2	0VA	D	501	30/30	0.92	0.19	1.92	29,30,33,34	0
2	0VA	A	501	30/30	0.91	0.20	1.91	31,33,35,36	0
2	0VA	E	501	30/30	0.89	0.24	1.49	30,32,36,38	0
3	IOD	D	503	1/1	0.97	0.12	-1.01	71,71,71,71	0
3	IOD	E	503	1/1	0.98	0.10	-1.19	70,70,70,70	0
3	IOD	B	503	1/1	0.99	0.06	-2.89	69,69,69,69	0
3	IOD	A	503	1/1	0.97	0.06	-2.99	65,65,65,65	0
3	IOD	E	504	1/1	-0.01	1.15	-	500,500,500,500	0
3	IOD	D	502	1/1	0.99	0.07	-	57,57,57,57	0
3	IOD	E	502	1/1	0.97	0.08	-	86,86,86,86	0
3	IOD	A	502	1/1	0.97	0.09	-	77,77,77,77	0
3	IOD	B	502	1/1	0.99	0.08	-	74,74,74,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.