



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2017 – 12:02 PM EDT

PDB ID : 5VDI
Title : Crystal Structure of Human Glycine Receptor alpha-3 Mutant N38Q Bound to AM-3607, Glycine, and Ivermectin
Authors : Shaffer, P.L.; Huang, X.; Chen, H.
Deposited on : 2017-04-03
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

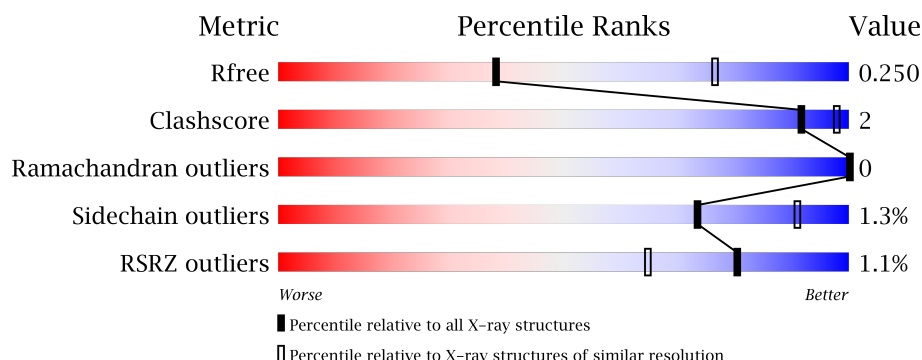
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	362	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	362	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	362	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>
1	D	362	<div> <div></div> <div> <div></div> <div>89%</div> <div>6%</div> <div>6%</div> </div> </div>
1	E	362	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>•</div> <div>7%</div> </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
3	GLY	D	402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14105 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 Glycine receptor subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2695	1759	431	485	20			
1	B	343	Total	C	N	O	S	0	0	0
			2714	1772	430	492	20			
1	C	338	Total	C	N	O	S	0	0	0
			2687	1755	425	487	20			
1	D	341	Total	C	N	O	S	0	0	0
			2720	1775	435	490	20			
1	E	338	Total	C	N	O	S	0	0	0
			2693	1758	428	487	20			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	ASN	engineered mutation	UNP O75311
A	310	ALA	-	linker	UNP O75311
A	311	GLY	-	linker	UNP O75311
A	312	THR	-	linker	UNP O75311
A	355	TRP	-	expression tag	UNP O75311
A	356	SER	-	expression tag	UNP O75311
A	357	HIS	-	expression tag	UNP O75311
A	358	PRO	-	expression tag	UNP O75311
A	359	GLN	-	expression tag	UNP O75311
A	360	PHE	-	expression tag	UNP O75311
A	361	GLU	-	expression tag	UNP O75311
A	362	LYS	-	expression tag	UNP O75311
B	38	GLN	ASN	engineered mutation	UNP O75311
B	310	ALA	-	linker	UNP O75311
B	311	GLY	-	linker	UNP O75311
B	312	THR	-	linker	UNP O75311
B	355	TRP	-	expression tag	UNP O75311
B	356	SER	-	expression tag	UNP O75311
B	357	HIS	-	expression tag	UNP O75311

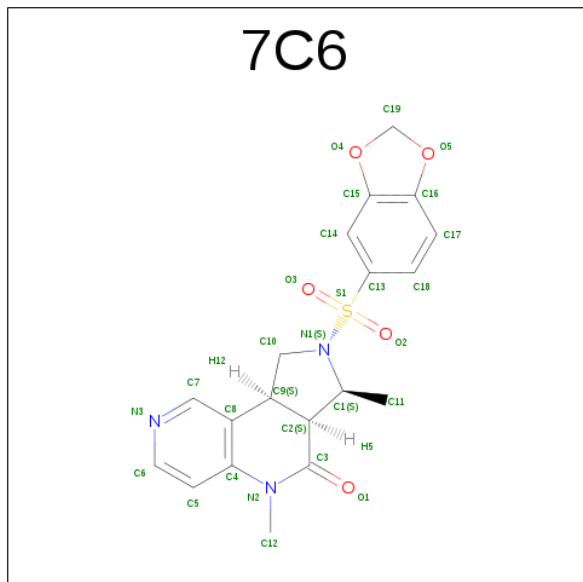
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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	PRO	-	expression tag	UNP O75311
B	359	GLN	-	expression tag	UNP O75311
B	360	PHE	-	expression tag	UNP O75311
B	361	GLU	-	expression tag	UNP O75311
B	362	LYS	-	expression tag	UNP O75311
C	38	GLN	ASN	engineered mutation	UNP O75311
C	310	ALA	-	linker	UNP O75311
C	311	GLY	-	linker	UNP O75311
C	312	THR	-	linker	UNP O75311
C	355	TRP	-	expression tag	UNP O75311
C	356	SER	-	expression tag	UNP O75311
C	357	HIS	-	expression tag	UNP O75311
C	358	PRO	-	expression tag	UNP O75311
C	359	GLN	-	expression tag	UNP O75311
C	360	PHE	-	expression tag	UNP O75311
C	361	GLU	-	expression tag	UNP O75311
C	362	LYS	-	expression tag	UNP O75311
D	38	GLN	ASN	engineered mutation	UNP O75311
D	310	ALA	-	linker	UNP O75311
D	311	GLY	-	linker	UNP O75311
D	312	THR	-	linker	UNP O75311
D	355	TRP	-	expression tag	UNP O75311
D	356	SER	-	expression tag	UNP O75311
D	357	HIS	-	expression tag	UNP O75311
D	358	PRO	-	expression tag	UNP O75311
D	359	GLN	-	expression tag	UNP O75311
D	360	PHE	-	expression tag	UNP O75311
D	361	GLU	-	expression tag	UNP O75311
D	362	LYS	-	expression tag	UNP O75311
E	38	GLN	ASN	engineered mutation	UNP O75311
E	310	ALA	-	linker	UNP O75311
E	311	GLY	-	linker	UNP O75311
E	312	THR	-	linker	UNP O75311
E	355	TRP	-	expression tag	UNP O75311
E	356	SER	-	expression tag	UNP O75311
E	357	HIS	-	expression tag	UNP O75311
E	358	PRO	-	expression tag	UNP O75311
E	359	GLN	-	expression tag	UNP O75311
E	360	PHE	-	expression tag	UNP O75311
E	361	GLU	-	expression tag	UNP O75311
E	362	LYS	-	expression tag	UNP O75311

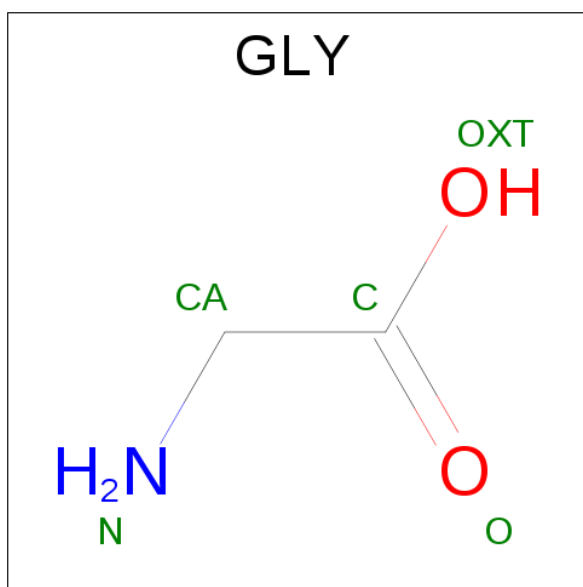
- Molecule 2 is (3S,3aS,9bS)-2-[(2H-1,3-benzodioxol-5-yl)sulfonyl]-3,5-dimethyl-1,2,3,3a,5,

9b-hexahydro-4H-pyrrolo[3,4-c][1,6]naphthyridin-4-one (three-letter code: 7C6) (formula: $C_{19}H_{19}N_3O_5S$).



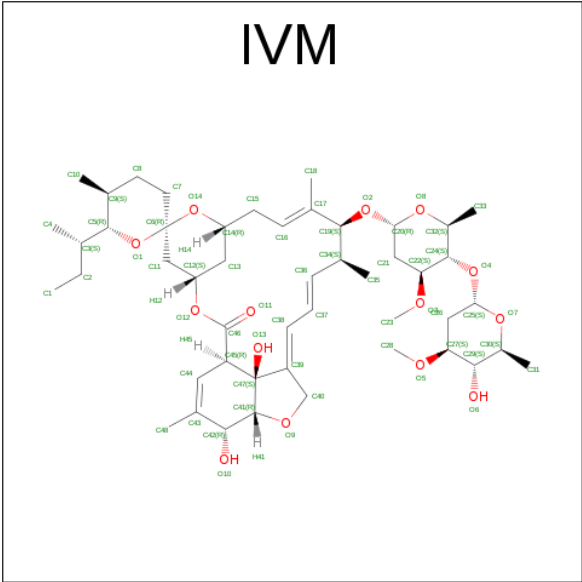
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	C	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	D	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
2	E	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		
3	E	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacyclooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			62	48	14		
4	B	1	Total	C	O	0	0
			62	48	14		
4	C	1	Total	C	O	0	0
			62	48	14		
4	D	1	Total	C	O	0	0
			62	48	14		
4	E	1	Total	C	O	0	0
			62	48	14		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

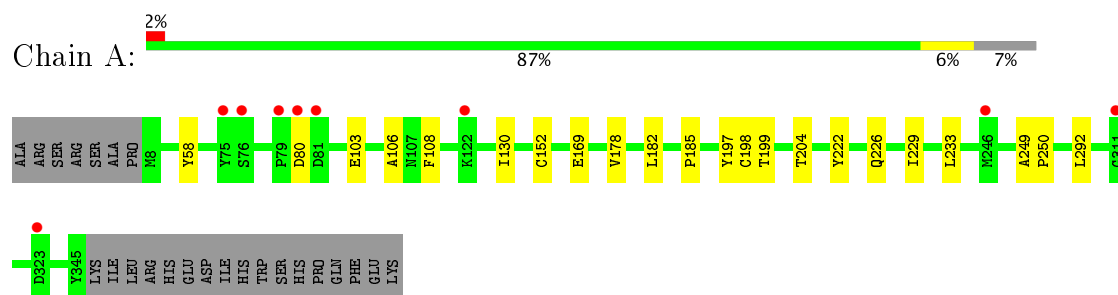
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	23	Total 23	O 23	0	0
6	C	31	Total 31	O 31	0	0
6	D	20	Total 20	O 20	0	0
6	E	17	Total 17	O 17	0	0

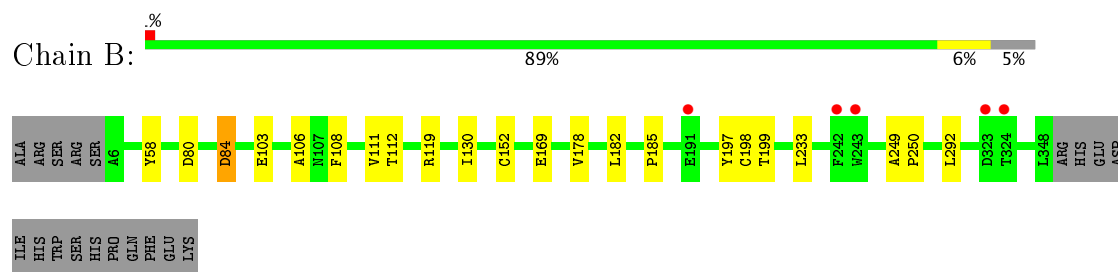
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

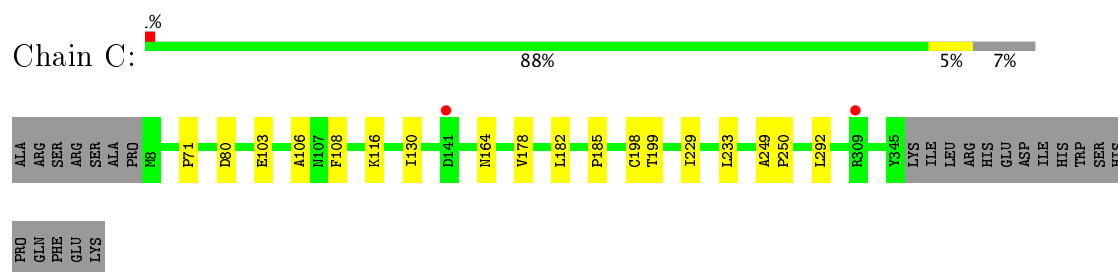
- Molecule 1: Glycine receptor subunit alpha-3



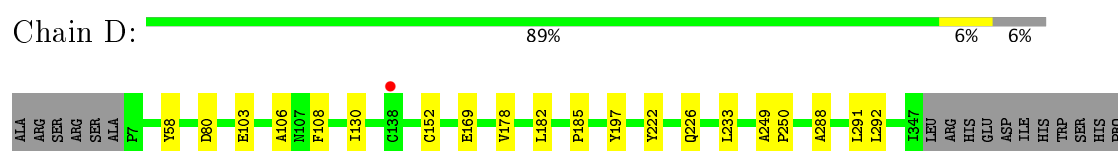
- Molecule 1: Glycine receptor subunit alpha-3



- Molecule 1: Glycine receptor subunit alpha-3

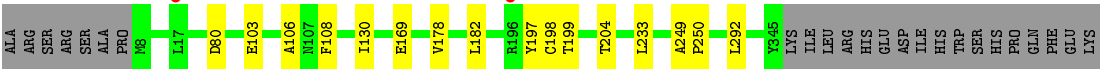
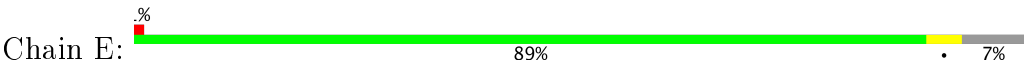


- Molecule 1: Glycine receptor subunit alpha-3



GLN
PHE
GLU
LYS

● Molecule 1: Glycine receptor subunit alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.01Å 136.00Å 191.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 47.91 – 3.08	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.10) 98.5 (47.91-3.08)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.256 0.229 , 0.250	Depositor DCC
R_{free} test set	1212 reflections (1.90%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	1.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IVM, ZN, 7C6

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	0.34	0/2766	0.53	0/3767
1	B	0.35	0/2786	0.54	1/3798 (0.0%)
1	C	0.34	0/2758	0.53	0/3758
1	D	0.33	0/2792	0.53	0/3801
1	E	0.33	0/2764	0.53	0/3765
All	All	0.34	0/13866	0.53	1/18889 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ASP	CB-CG-OD1	7.83	125.35	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2695	0	2645	10	0
1	B	2714	0	2645	9	0
1	C	2687	0	2627	9	0
1	D	2720	0	2672	9	0
1	E	2693	0	2638	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	0	0	0
2	B	28	0	0	0	0
2	C	28	0	0	0	0
2	D	28	0	0	0	0
2	E	28	0	0	0	0
3	A	5	0	2	1	0
3	B	5	0	2	1	0
3	C	5	0	2	0	0
3	D	5	0	2	1	0
3	E	5	0	2	1	0
4	A	62	0	74	1	0
4	B	62	0	74	2	0
4	C	62	0	74	2	0
4	D	62	0	74	4	0
4	E	62	0	74	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	25	0	0	0	0
6	B	23	0	0	0	0
6	C	31	0	0	3	0
6	D	20	0	0	1	0
6	E	17	0	0	0	0
All	All	14105	0	13607	52	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 2.

All (52) 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)
4:C:403:IVM:H33	4:C:403:IVM:H25	1.43	1.00
4:C:403:IVM:C33	4:C:403:IVM:H25	2.17	0.75
1:A:229:ILE:HD11	4:E:403:IVM:H23B	1.70	0.73
4:B:403:IVM:H23B	1:C:229:ILE:HD11	1.73	0.69
3:B:402:GLY:N	6:C:603:HOH:O	2.36	0.57
1:E:204:THR:OG1	3:E:402:GLY:OXT	2.16	0.56
3:D:402:GLY:N	6:D:501:HOH:O	2.38	0.56
4:B:403:IVM:H33	4:B:403:IVM:H30	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:GLU:OE2	1:D:197:TYR:OH	2.22	0.53
1:A:222:TYR:CE2	1:A:226:GLN:HG3	2.43	0.52
1:A:169:GLU:OE2	1:A:197:TYR:OH	2.22	0.52
1:E:103:GLU:HG3	1:E:106:ALA:HB2	1.92	0.52
1:C:103:GLU:HG3	1:C:106:ALA:HB2	1.92	0.51
1:B:103:GLU:HG3	1:B:106:ALA:HB2	1.93	0.51
1:D:103:GLU:HG3	1:D:106:ALA:HB2	1.92	0.50
4:A:403:IVM:C33	4:A:403:IVM:H25	2.42	0.50
1:A:103:GLU:HG3	1:A:106:ALA:HB2	1.93	0.49
1:B:84:ASP:OD1	1:B:119:ARG:NE	2.42	0.47
1:D:288:ALA:HB1	4:D:403:IVM:H18B	1.95	0.47
1:C:71:PRO:HG2	6:C:629:HOH:O	2.14	0.47
1:B:169:GLU:OE2	1:B:197:TYR:OH	2.25	0.46
1:B:249:ALA:N	1:B:250:PRO:HD2	2.31	0.46
1:D:178:VAL:HG13	1:D:182:LEU:HD23	1.98	0.45
1:E:178:VAL:HG13	1:E:182:LEU:HD23	1.97	0.45
1:C:178:VAL:HG13	1:C:182:LEU:HD23	1.99	0.45
1:A:249:ALA:N	1:A:250:PRO:HD2	2.31	0.45
1:D:249:ALA:N	1:D:250:PRO:HD2	2.31	0.45
1:E:249:ALA:N	1:E:250:PRO:HD2	2.31	0.45
1:C:249:ALA:N	1:C:250:PRO:HD2	2.32	0.45
4:D:403:IVM:H33	4:D:403:IVM:H25	1.98	0.45
1:E:169:GLU:OE2	1:E:197:TYR:OH	2.24	0.45
1:C:108:PHE:CD1	1:C:130:ILE:HD11	2.52	0.45
1:B:178:VAL:HG13	1:B:182:LEU:HD23	1.98	0.44
1:A:178:VAL:HG13	1:A:182:LEU:HD23	1.98	0.44
1:A:204:THR:OG1	3:A:402:GLY:O	2.25	0.44
4:D:403:IVM:H25	4:D:403:IVM:C33	2.48	0.44
1:E:108:PHE:CD1	1:E:130:ILE:HD11	2.53	0.44
1:B:108:PHE:CD1	1:B:130:ILE:HD11	2.54	0.43
1:C:164:ASN:HB3	6:C:625:HOH:O	2.17	0.43
1:A:108:PHE:CD1	1:A:130:ILE:HD11	2.54	0.42
1:D:108:PHE:CD1	1:D:130:ILE:HD11	2.55	0.42
1:C:198:CYS:O	1:C:199:THR:C	2.58	0.42
1:E:198:CYS:O	1:E:199:THR:C	2.59	0.42
1:A:198:CYS:O	1:A:199:THR:C	2.58	0.41
1:B:58:TYR:CE1	1:B:152:CYS:HB3	2.56	0.41
1:D:222:TYR:CE1	1:D:226:GLN:HG3	2.56	0.41
1:D:291:LEU:HD23	4:D:403:IVM:C46	2.50	0.41
1:B:111:VAL:HA	1:B:112:THR:HA	1.91	0.41
1:C:116:LYS:HE2	1:C:130:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:CYS:O	1:B:199:THR:C	2.60	0.40
1:A:58:TYR:CE1	1:A:152:CYS:HB3	2.56	0.40
1:D:58:TYR:CE1	1:D:152:CYS:HB3	2.56	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	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
1	B	341/362 (94%)	331 (97%)	10 (3%)	0	100	100
1	C	336/362 (93%)	327 (97%)	9 (3%)	0	100	100
1	D	339/362 (94%)	330 (97%)	9 (3%)	0	100	100
1	E	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
All	All	1688/1810 (93%)	1647 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/326 (90%)	290 (99%)	4 (1%)	71	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	294/326 (90%)	290 (99%)	4 (1%)	71	90
1	C	293/326 (90%)	289 (99%)	4 (1%)	71	90
1	D	297/326 (91%)	293 (99%)	4 (1%)	73	91
1	E	294/326 (90%)	291 (99%)	3 (1%)	80	92
All	All	1472/1630 (90%)	1453 (99%)	19 (1%)	73	91

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	185	PRO
1	A	233	LEU
1	A	292	LEU
1	B	80	ASP
1	B	185	PRO
1	B	233	LEU
1	B	292	LEU
1	C	80	ASP
1	C	185	PRO
1	C	233	LEU
1	C	292	LEU
1	D	80	ASP
1	D	185	PRO
1	D	233	LEU
1	D	292	LEU
1	E	80	ASP
1	E	233	LEU
1	E	292	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN

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 ⓘ

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	7C6	A	401	-	30,32,32	1.79	5 (16%)	37,50,50	1.91	8 (21%)
3	GLY	A	402	-	1,4,4	0.80	0	0,4,4	0.00	-
4	IVM	A	403	-	66,68,68	1.73	7 (10%)	77,102,102	1.63	13 (16%)
2	7C6	B	401	-	30,32,32	1.92	5 (16%)	37,50,50	1.88	8 (21%)
3	GLY	B	402	-	1,4,4	0.72	0	0,4,4	0.00	-
4	IVM	B	403	-	66,68,68	1.81	7 (10%)	77,102,102	1.38	10 (12%)
2	7C6	C	401	-	30,32,32	1.96	6 (20%)	37,50,50	1.81	9 (24%)
3	GLY	C	402	-	1,4,4	0.89	0	0,4,4	0.00	-
4	IVM	C	403	-	66,68,68	1.87	11 (16%)	77,102,102	1.74	16 (20%)
2	7C6	D	401	-	30,32,32	1.79	5 (16%)	37,50,50	1.95	10 (27%)
3	GLY	D	402	-	1,4,4	0.76	0	0,4,4	0.00	-
4	IVM	D	403	-	66,68,68	1.85	11 (16%)	77,102,102	1.54	16 (20%)
2	7C6	E	401	-	30,32,32	1.74	4 (13%)	37,50,50	1.86	9 (24%)
3	GLY	E	402	-	1,4,4	0.82	0	0,4,4	0.00	-
4	IVM	E	403	-	66,68,68	1.83	9 (13%)	77,102,102	1.37	16 (20%)

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	7C6	A	401	-	-	0/12/50/50	0/5/5/5
3	GLY	A	402	-	-	0/0/2/2	0/0/0/0
4	IVM	A	403	-	-	0/44/141/141	0/5/7/7
2	7C6	B	401	-	-	0/12/50/50	0/5/5/5
3	GLY	B	402	-	-	0/0/2/2	0/0/0/0
4	IVM	B	403	-	-	0/44/141/141	1/5/7/7
2	7C6	C	401	-	-	0/12/50/50	0/5/5/5
3	GLY	C	402	-	-	0/0/2/2	0/0/0/0
4	IVM	C	403	-	-	0/44/141/141	0/5/7/7
2	7C6	D	401	-	-	0/12/50/50	0/5/5/5
3	GLY	D	402	-	-	0/0/2/2	0/0/0/0
4	IVM	D	403	-	-	0/44/141/141	0/5/7/7
2	7C6	E	401	-	-	0/12/50/50	0/5/5/5
3	GLY	E	402	-	-	0/0/2/2	0/0/0/0
4	IVM	E	403	-	-	0/44/141/141	0/5/7/7

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	403	IVM	C40-C39	-5.83	1.39	1.50
4	C	403	IVM	C40-C39	-5.77	1.39	1.50
4	E	403	IVM	C15-C16	-5.58	1.39	1.50
4	D	403	IVM	C40-C39	-5.57	1.40	1.50
4	D	403	IVM	C15-C16	-5.55	1.39	1.50
4	A	403	IVM	C15-C16	-5.42	1.39	1.50
4	B	403	IVM	C40-C39	-5.39	1.40	1.50
4	A	403	IVM	C40-C39	-5.36	1.40	1.50
4	C	403	IVM	C15-C16	-5.31	1.39	1.50
4	B	403	IVM	C15-C16	-5.30	1.39	1.50
2	B	401	7C6	C13-S1	-3.85	1.70	1.76
2	C	401	7C6	C13-S1	-3.84	1.70	1.76
2	D	401	7C6	C13-S1	-2.57	1.72	1.76
2	D	401	7C6	O5-C16	-2.23	1.35	1.38
2	B	401	7C6	O5-C16	-2.18	1.35	1.38
2	C	401	7C6	O5-C16	-2.08	1.35	1.38
4	C	403	IVM	C21-C22	2.01	1.55	1.52
2	E	401	7C6	C2-C3	2.03	1.54	1.51
4	D	403	IVM	C26-C25	2.06	1.55	1.51
4	A	403	IVM	C21-C22	2.07	1.56	1.52
4	D	403	IVM	C41-C42	2.08	1.54	1.51
2	D	401	7C6	S1-N1	2.12	1.66	1.63
4	E	403	IVM	C41-C42	2.16	1.55	1.51
4	B	403	IVM	C45-C44	2.20	1.53	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	7C6	C2-C3	2.21	1.54	1.51
4	D	403	IVM	O9-C40	2.31	1.47	1.43
4	C	403	IVM	O7-C25	2.32	1.48	1.42
4	D	403	IVM	C26-C27	2.38	1.56	1.52
4	C	403	IVM	C41-C42	2.45	1.55	1.51
4	C	403	IVM	C11-C12	2.47	1.56	1.51
4	E	403	IVM	O5-C27	2.48	1.50	1.43
4	C	403	IVM	C45-C44	2.53	1.54	1.51
4	E	403	IVM	C26-C27	2.54	1.57	1.52
2	A	401	7C6	C2-C3	2.55	1.55	1.51
2	B	401	7C6	C2-C3	2.56	1.55	1.51
2	A	401	7C6	C8-C9	2.58	1.56	1.52
4	D	403	IVM	O5-C27	2.67	1.50	1.43
4	A	403	IVM	C45-C44	2.69	1.54	1.51
2	A	401	7C6	S1-N1	2.70	1.67	1.63
4	D	403	IVM	C45-C44	2.75	1.54	1.51
4	B	403	IVM	C41-C42	2.90	1.56	1.51
2	C	401	7C6	S1-N1	3.06	1.67	1.63
4	E	403	IVM	C45-C44	3.21	1.55	1.51
4	C	403	IVM	O9-C40	3.50	1.49	1.43
2	E	401	7C6	S1-N1	3.69	1.68	1.63
4	A	403	IVM	C38-C39	3.74	1.38	1.33
4	C	403	IVM	C38-C39	4.12	1.39	1.33
4	E	403	IVM	C38-C39	4.15	1.39	1.33
4	D	403	IVM	C38-C39	4.34	1.39	1.33
4	C	403	IVM	C16-C17	4.42	1.38	1.33
4	B	403	IVM	C38-C39	4.53	1.39	1.33
4	A	403	IVM	C16-C17	4.80	1.39	1.33
4	D	403	IVM	C16-C17	5.04	1.39	1.33
4	E	403	IVM	C16-C17	5.15	1.39	1.33
2	E	401	7C6	O2-S1	5.27	1.50	1.43
4	B	403	IVM	C16-C17	5.27	1.40	1.33
2	E	401	7C6	O3-S1	5.29	1.50	1.43
2	D	401	7C6	O2-S1	5.33	1.50	1.43
4	C	403	IVM	C44-C43	5.36	1.39	1.33
2	C	401	7C6	O2-S1	5.49	1.50	1.43
2	A	401	7C6	O3-S1	5.53	1.50	1.43
4	B	403	IVM	C44-C43	5.54	1.40	1.33
2	A	401	7C6	O2-S1	5.56	1.50	1.43
4	D	403	IVM	C44-C43	5.69	1.40	1.33
4	E	403	IVM	C44-C43	5.80	1.40	1.33
2	B	401	7C6	O2-S1	5.87	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	IVM	C44-C43	5.93	1.40	1.33
2	B	401	7C6	O3-S1	6.05	1.51	1.43
2	C	401	7C6	O3-S1	6.16	1.51	1.43
2	D	401	7C6	O3-S1	6.22	1.51	1.43

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	7C6	O2-S1-O3	-5.79	109.73	119.46
2	D	401	7C6	O2-S1-O3	-5.75	109.78	119.46
2	A	401	7C6	O2-S1-O3	-5.61	110.03	119.46
2	D	401	7C6	C10-N1-S1	-4.83	109.18	118.81
2	B	401	7C6	O2-S1-O3	-4.73	111.50	119.46
2	D	401	7C6	C7-C8-C9	-4.73	119.84	124.98
2	C	401	7C6	O2-S1-O3	-4.64	111.66	119.46
4	C	403	IVM	C26-C27-C29	-4.42	104.17	110.75
4	A	403	IVM	C13-C14-C15	-4.41	107.12	113.31
4	A	403	IVM	O7-C30-C29	-4.24	102.64	109.62
4	A	403	IVM	C26-C27-C29	-4.18	104.53	110.75
2	B	401	7C6	C7-C8-C9	-4.13	120.49	124.98
2	B	401	7C6	C10-N1-S1	-4.06	110.70	118.81
2	A	401	7C6	C7-C8-C9	-3.95	120.69	124.98
2	E	401	7C6	C7-C8-C9	-3.87	120.78	124.98
4	D	403	IVM	C22-C24-C32	-3.86	104.06	110.49
2	C	401	7C6	C7-C8-C9	-3.75	120.90	124.98
4	C	403	IVM	C13-C14-C15	-3.48	108.42	113.31
4	C	403	IVM	C38-C37-C36	-3.36	115.81	124.55
4	A	403	IVM	C37-C38-C39	-3.34	119.63	130.18
2	C	401	7C6	O5-C19-O4	-3.32	102.92	108.10
4	E	403	IVM	C3-C5-C9	-3.23	110.66	116.47
4	D	403	IVM	O14-C6-C11	-3.20	106.40	110.71
2	E	401	7C6	O5-C19-O4	-3.18	103.14	108.10
2	B	401	7C6	O5-C19-O4	-3.17	103.16	108.10
2	C	401	7C6	C10-N1-S1	-3.15	112.52	118.81
2	A	401	7C6	C10-N1-S1	-3.11	112.61	118.81
4	D	403	IVM	C48-C43-C44	-3.05	117.11	123.68
4	B	403	IVM	C37-C38-C39	-3.02	120.65	130.18
2	A	401	7C6	O5-C19-O4	-2.90	103.57	108.10
4	C	403	IVM	O7-C30-C29	-2.86	104.92	109.62
4	C	403	IVM	C3-C5-C9	-2.79	111.46	116.47
4	D	403	IVM	C3-C5-C9	-2.70	111.62	116.47
4	E	403	IVM	C37-C38-C39	-2.67	121.73	130.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	7C6	C10-N1-S1	-2.56	113.69	118.81
4	D	403	IVM	C26-C27-C29	-2.47	107.07	110.75
4	D	403	IVM	C38-C37-C36	-2.45	118.17	124.55
4	E	403	IVM	C38-C37-C36	-2.42	118.25	124.55
4	A	403	IVM	O11-C46-C45	-2.40	120.69	124.99
4	B	403	IVM	O8-C20-C21	-2.40	107.13	110.83
4	D	403	IVM	C37-C38-C39	-2.38	122.68	130.18
4	C	403	IVM	O11-C46-C45	-2.35	120.78	124.99
4	C	403	IVM	C48-C43-C44	-2.33	118.67	123.68
4	B	403	IVM	C38-C37-C36	-2.32	118.51	124.55
4	E	403	IVM	O11-C46-C45	-2.28	120.91	124.99
4	A	403	IVM	C38-C37-C36	-2.27	118.63	124.55
4	E	403	IVM	C48-C43-C44	-2.25	118.83	123.68
4	E	403	IVM	C6-C11-C12	-2.22	108.02	111.54
4	B	403	IVM	C34-C36-C37	-2.21	120.89	126.06
2	B	401	7C6	C10-N1-C1	-2.20	107.75	110.66
4	E	403	IVM	C13-C14-C15	-2.20	110.22	113.31
2	D	401	7C6	C10-N1-C1	-2.17	107.80	110.66
4	A	403	IVM	C3-C5-C9	-2.16	112.58	116.47
2	B	401	7C6	C8-C7-N3	-2.15	120.01	124.28
2	D	401	7C6	O5-C19-O4	-2.14	104.75	108.10
4	E	403	IVM	O14-C6-C11	-2.04	107.96	110.71
2	D	401	7C6	C8-C7-N3	-2.04	120.23	124.28
2	C	401	7C6	C8-C7-N3	-2.03	120.24	124.28
4	D	403	IVM	O7-C30-C29	-2.02	106.30	109.62
4	B	403	IVM	C48-C43-C44	-2.02	119.34	123.68
4	B	403	IVM	O11-C46-C45	-2.01	121.40	124.99
4	E	403	IVM	O12-C12-C11	2.09	112.85	107.61
2	E	401	7C6	O5-C16-C17	2.10	131.40	127.86
4	C	403	IVM	O7-C30-C31	2.11	111.15	106.69
4	E	403	IVM	C18-C17-C19	2.11	119.26	115.69
4	D	403	IVM	O4-C24-C32	2.12	112.46	106.72
4	A	403	IVM	C33-C32-C24	2.15	116.67	113.36
2	E	401	7C6	C9-C10-N1	2.17	105.94	103.24
4	A	403	IVM	O7-C30-C31	2.18	111.30	106.69
4	E	403	IVM	C8-C9-C5	2.24	111.83	108.55
2	D	401	7C6	C9-C10-N1	2.24	106.03	103.24
4	E	403	IVM	O7-C30-C31	2.25	111.45	106.69
4	A	403	IVM	C18-C17-C19	2.25	119.50	115.69
4	E	403	IVM	O5-C27-C29	2.28	114.02	108.67
4	B	403	IVM	O7-C30-C31	2.30	111.56	106.69
2	D	401	7C6	C13-S1-N1	2.31	111.40	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	IVM	O8-C32-C33	2.33	111.63	106.69
4	D	403	IVM	C48-C43-C42	2.36	120.93	116.47
2	E	401	7C6	C6-N3-C7	2.37	120.99	116.83
4	C	403	IVM	O8-C32-C24	2.45	113.77	109.14
4	D	403	IVM	O4-C25-C26	2.46	112.82	108.47
4	E	403	IVM	C8-C7-C6	2.49	114.74	111.74
4	E	403	IVM	O14-C14-C15	2.52	108.40	106.05
2	A	401	7C6	O5-C16-C17	2.59	132.24	127.86
2	A	401	7C6	C13-S1-N1	2.60	111.90	107.37
2	A	401	7C6	C6-N3-C7	2.61	121.41	116.83
2	D	401	7C6	O4-C15-C14	2.62	131.34	127.86
2	C	401	7C6	O4-C15-C14	2.62	131.34	127.86
2	B	401	7C6	O4-C15-C14	2.63	131.36	127.86
4	C	403	IVM	C18-C17-C19	2.64	120.14	115.69
4	D	403	IVM	C8-C9-C5	2.71	112.53	108.55
2	C	401	7C6	C9-C10-N1	2.71	106.63	103.24
4	B	403	IVM	O8-C32-C24	2.75	114.33	109.14
4	D	403	IVM	C8-C7-C6	2.78	115.08	111.74
4	C	403	IVM	O4-C24-C32	2.81	114.32	106.72
2	E	401	7C6	O4-C15-C14	2.86	131.66	127.86
2	D	401	7C6	C6-N3-C7	2.90	121.91	116.83
4	C	403	IVM	C8-C9-C5	2.94	112.88	108.55
2	C	401	7C6	C6-N3-C7	3.05	122.18	116.83
4	E	403	IVM	O12-C46-C45	3.08	116.42	111.35
2	A	401	7C6	O4-C15-C14	3.15	132.04	127.86
2	B	401	7C6	C6-N3-C7	3.18	122.41	116.83
4	A	403	IVM	O5-C27-C29	3.49	116.85	108.67
2	C	401	7C6	C13-S1-N1	3.50	113.47	107.37
4	C	403	IVM	O14-C14-C13	3.59	115.72	108.85
4	C	403	IVM	O5-C27-C29	3.63	117.18	108.67
4	D	403	IVM	O12-C46-C45	3.69	117.44	111.35
4	D	403	IVM	O5-C27-C29	3.76	117.47	108.67
2	E	401	7C6	C13-S1-N1	3.76	113.94	107.37
4	B	403	IVM	O12-C46-C45	3.79	117.59	111.35
4	C	403	IVM	O12-C46-C45	3.79	117.59	111.35
4	A	403	IVM	O14-C14-C15	3.87	109.65	106.05
4	A	403	IVM	O12-C46-C45	4.10	118.11	111.35
4	C	403	IVM	O14-C14-C15	4.28	110.04	106.05
4	B	403	IVM	O14-C14-C15	5.40	111.08	106.05

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	IVM	C5-C6-C7-C8-C9-O1

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GLY	1	0
4	A	403	IVM	1	0
3	B	402	GLY	1	0
4	B	403	IVM	2	0
4	C	403	IVM	2	0
3	D	402	GLY	1	0
4	D	403	IVM	4	0
3	E	402	GLY	1	0
4	E	403	IVM	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	338/362 (93%)	-0.21	9 (2%) 55 30	40, 63, 90, 108	0
1	B	343/362 (94%)	-0.18	5 (1%) 74 54	41, 58, 89, 110	0
1	C	338/362 (93%)	-0.27	2 (0%) 89 77	41, 56, 83, 103	0
1	D	341/362 (94%)	-0.28	1 (0%) 93 86	44, 63, 77, 101	0
1	E	338/362 (93%)	-0.15	2 (0%) 89 77	45, 68, 91, 115	0
All	All	1698/1810 (93%)	-0.22	19 (1%) 80 65	40, 63, 88, 115	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	PRO	5.1
1	A	81	ASP	4.4
1	A	76	SER	3.6
1	A	80	ASP	3.2
1	B	191	GLU	2.8
1	A	122	LYS	2.7
1	A	311	GLY	2.5
1	C	141	ASP	2.4
1	D	138	CYS	2.3
1	C	309	ARG	2.3
1	B	323	ASP	2.3
1	B	324	THR	2.3
1	A	323	ASP	2.3
1	B	243	TRP	2.1
1	A	246	MET	2.1
1	E	17	LEU	2.1
1	B	242	PHE	2.1
1	A	75	TYR	2.0
1	E	196	ARG	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
3	GLY	D	402	5/5	0.98	0.32	5.67	46,47,47,48	0
3	GLY	E	402	5/5	0.95	0.35	1.70	54,54,54,55	0
4	IVM	B	403	62/62	0.90	0.25	1.66	57,66,87,88	0
3	GLY	B	402	5/5	0.97	0.23	1.59	44,44,45,45	0
4	IVM	E	403	62/62	0.90	0.27	0.90	61,72,102,106	0
4	IVM	D	403	62/62	0.92	0.24	0.72	62,68,100,103	0
4	IVM	A	403	62/62	0.93	0.20	0.32	60,67,118,126	0
4	IVM	C	403	62/62	0.92	0.21	0.22	59,63,99,104	0
3	GLY	C	402	5/5	0.98	0.21	0.17	52,52,53,53	0
2	7C6	D	401	28/28	0.96	0.25	0.08	65,68,71,72	0
2	7C6	E	401	28/28	0.92	0.25	-0.02	65,68,70,71	0
2	7C6	A	401	28/28	0.96	0.23	-0.11	42,46,49,49	0
2	7C6	B	401	28/28	0.97	0.18	-0.61	50,53,56,57	0
2	7C6	C	401	28/28	0.97	0.14	-1.35	48,49,52,52	0
3	GLY	A	402	5/5	0.97	0.15	-1.56	42,42,43,43	0
5	ZN	E	404	1/1	0.73	0.34	-	88,88,88,88	1
5	ZN	C	404	1/1	0.88	0.42	-	79,79,79,79	1
5	ZN	A	404	1/1	0.91	0.30	-	66,66,66,66	1
5	ZN	B	404	1/1	0.82	0.30	-	71,71,71,71	1
5	ZN	D	404	1/1	0.66	0.43	-	106,106,106,106	1

6.5 Other polymers [i](#)

There are no such residues in this entry.