



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:22 AM UTC

PDB ID : 2PDO / pdb_00002pdo
Title : Crystal Structure of the Putative Acetyltransferase of GNAT Family from *Shigella flexneri*
Authors : Kim, Y.; Li, H.; Holzle, D.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-04-01
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

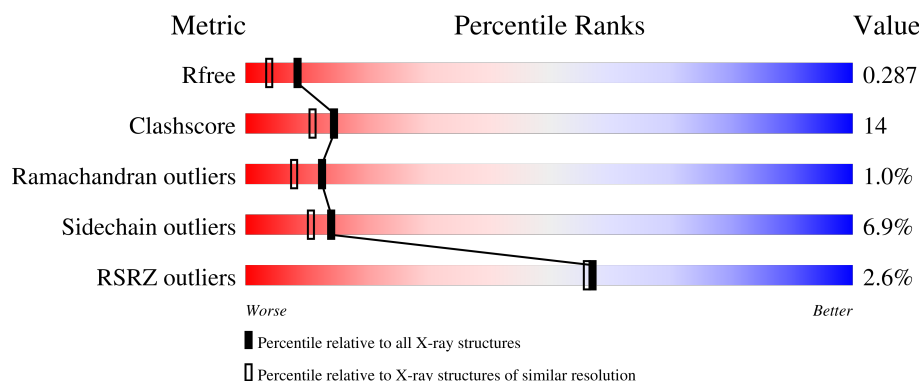
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	144	 3% 74% 23% ..
1	B	144	 3% 71% 25% ..
1	C	144	 3% 72% 22% ..
1	D	144	 2% 69% 26% ..
1	E	144	 3% 66% 26% 6% .

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Mol	Chain	Length	Quality of chain
1	F	144	
1	G	144	
1	H	144	

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	ACY	B	607	-	X	X	-
4	EDO	D	608	-	-	X	-
4	EDO	F	609	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10253 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 Acetyltransferase ypeA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	Se	0	9	0
			1209	755	211	234	2	7			
1	B	141	Total	C	N	O	S	Se	0	9	0
			1229	769	216	236	2	6			
1	C	140	Total	C	N	O	S	Se	0	6	0
			1183	740	211	224	2	6			
1	D	142	Total	C	N	O	S	Se	0	7	0
			1215	759	217	231	2	6			
1	E	140	Total	C	N	O	S	Se	0	4	0
			1167	730	205	224	2	6			
1	F	141	Total	C	N	O	S	Se	0	7	0
			1203	750	218	227	2	6			
1	G	138	Total	C	N	O	S	Se	0	11	0
			1218	758	219	233	2	6			
1	H	140	Total	C	N	O	S	Se	0	8	0
			1201	748	213	232	2	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	UNP P63422
A	-1	ASN	-	cloning artifact	UNP P63422
A	0	ALA	-	cloning artifact	UNP P63422
A	1	MSE	MET	modified residue	UNP P63422
A	32	MSE	MET	modified residue	UNP P63422
A	38	MSE	MET	modified residue	UNP P63422
A	59	MSE	MET	modified residue	UNP P63422
A	113	MSE	MET	modified residue	UNP P63422
A	117	MSE	MET	modified residue	UNP P63422
B	-2	SER	-	cloning artifact	UNP P63422
B	-1	ASN	-	cloning artifact	UNP P63422
B	0	ALA	-	cloning artifact	UNP P63422
B	1	MSE	MET	modified residue	UNP P63422

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	MSE	MET	modified residue	UNP P63422
B	38	MSE	MET	modified residue	UNP P63422
B	59	MSE	MET	modified residue	UNP P63422
B	113	MSE	MET	modified residue	UNP P63422
B	117	MSE	MET	modified residue	UNP P63422
C	-2	SER	-	cloning artifact	UNP P63422
C	-1	ASN	-	cloning artifact	UNP P63422
C	0	ALA	-	cloning artifact	UNP P63422
C	1	MSE	MET	modified residue	UNP P63422
C	32	MSE	MET	modified residue	UNP P63422
C	38	MSE	MET	modified residue	UNP P63422
C	59	MSE	MET	modified residue	UNP P63422
C	113	MSE	MET	modified residue	UNP P63422
C	117	MSE	MET	modified residue	UNP P63422
D	-2	SER	-	cloning artifact	UNP P63422
D	-1	ASN	-	cloning artifact	UNP P63422
D	0	ALA	-	cloning artifact	UNP P63422
D	1	MSE	MET	modified residue	UNP P63422
D	32	MSE	MET	modified residue	UNP P63422
D	38	MSE	MET	modified residue	UNP P63422
D	59	MSE	MET	modified residue	UNP P63422
D	113	MSE	MET	modified residue	UNP P63422
D	117	MSE	MET	modified residue	UNP P63422
E	-2	SER	-	cloning artifact	UNP P63422
E	-1	ASN	-	cloning artifact	UNP P63422
E	0	ALA	-	cloning artifact	UNP P63422
E	1	MSE	MET	modified residue	UNP P63422
E	32	MSE	MET	modified residue	UNP P63422
E	38	MSE	MET	modified residue	UNP P63422
E	59	MSE	MET	modified residue	UNP P63422
E	113	MSE	MET	modified residue	UNP P63422
E	117	MSE	MET	modified residue	UNP P63422
F	-2	SER	-	cloning artifact	UNP P63422
F	-1	ASN	-	cloning artifact	UNP P63422
F	0	ALA	-	cloning artifact	UNP P63422
F	1	MSE	MET	modified residue	UNP P63422
F	32	MSE	MET	modified residue	UNP P63422
F	38	MSE	MET	modified residue	UNP P63422
F	59	MSE	MET	modified residue	UNP P63422
F	113	MSE	MET	modified residue	UNP P63422
F	117	MSE	MET	modified residue	UNP P63422
G	-2	SER	-	cloning artifact	UNP P63422

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ASN	-	cloning artifact	UNP P63422
G	0	ALA	-	cloning artifact	UNP P63422
G	1	MSE	MET	modified residue	UNP P63422
G	32	MSE	MET	modified residue	UNP P63422
G	38	MSE	MET	modified residue	UNP P63422
G	59	MSE	MET	modified residue	UNP P63422
G	113	MSE	MET	modified residue	UNP P63422
G	117	MSE	MET	modified residue	UNP P63422
H	-2	SER	-	cloning artifact	UNP P63422
H	-1	ASN	-	cloning artifact	UNP P63422
H	0	ALA	-	cloning artifact	UNP P63422
H	1	MSE	MET	modified residue	UNP P63422
H	32	MSE	MET	modified residue	UNP P63422
H	38	MSE	MET	modified residue	UNP P63422
H	59	MSE	MET	modified residue	UNP P63422
H	113	MSE	MET	modified residue	UNP P63422
H	117	MSE	MET	modified residue	UNP P63422

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

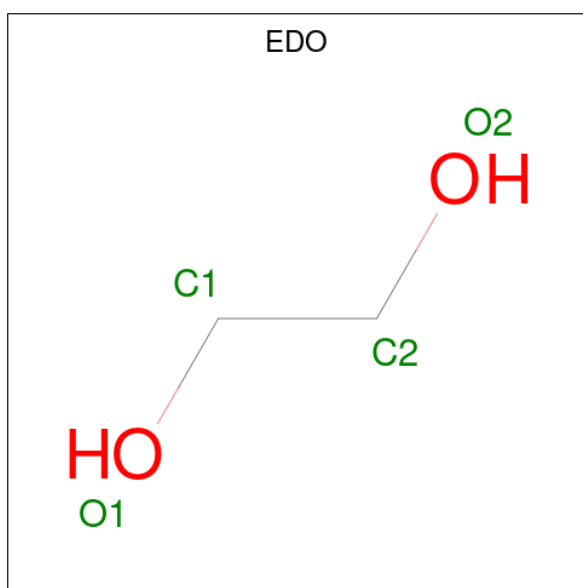
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0
2	E	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

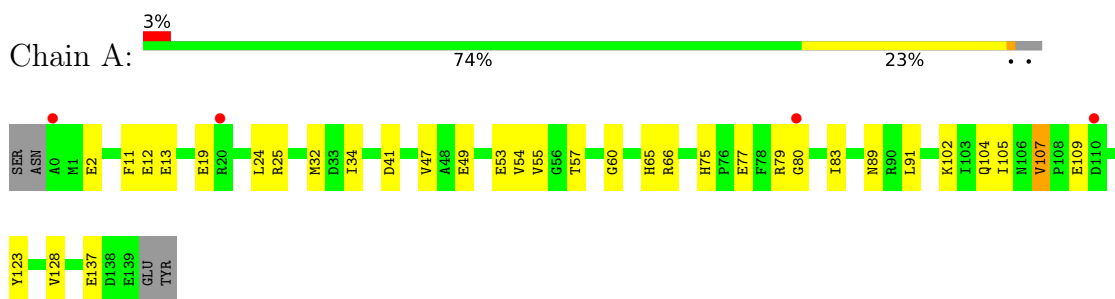
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	76	Total O 76 76	0	0
5	B	73	Total O 73 73	0	0
5	C	64	Total O 64 64	0	0
5	D	73	Total O 73 73	0	0
5	E	66	Total O 66 66	0	0
5	F	74	Total O 74 74	0	0
5	G	67	Total O 67 67	0	0
5	H	94	Total O 94 94	0	0

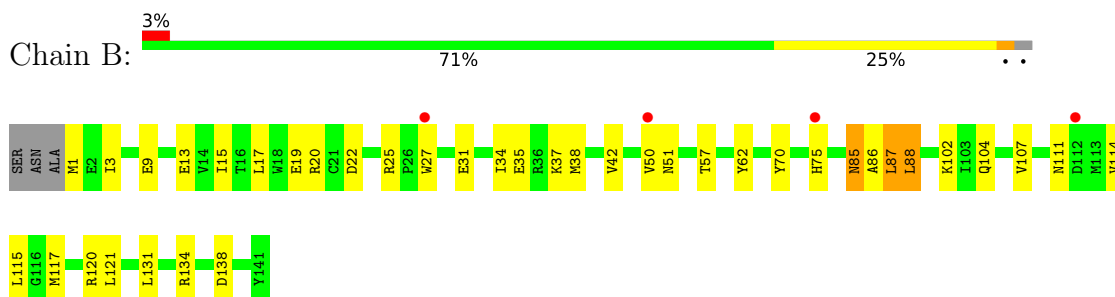
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

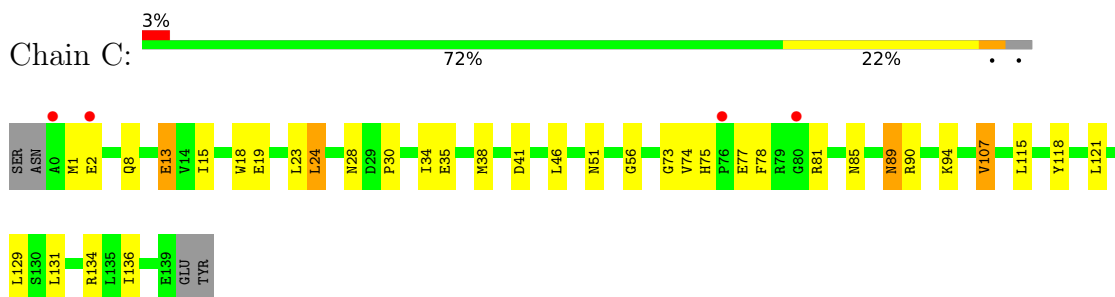
- Molecule 1: Acetyltransferase ypeA



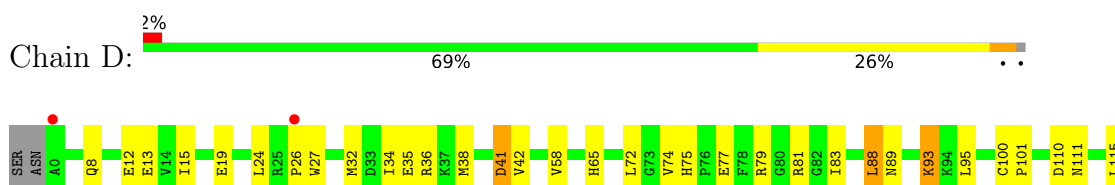
- Molecule 1: Acetyltransferase ypeA



- Molecule 1: Acetyltransferase ypeA



- Molecule 1: Acetyltransferase ypeA

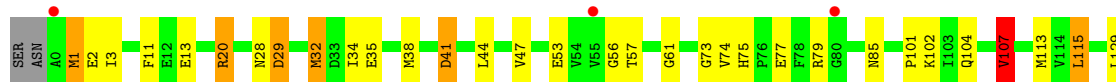




- Molecule 1: Acetyltransferase ypeA



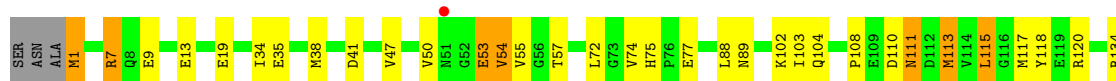
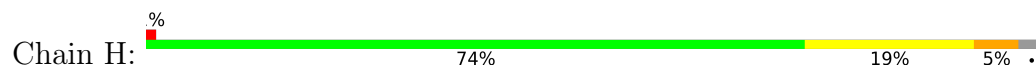
- Molecule 1: Acetyltransferase ypeA



- Molecule 1: Acetyltransferase ypeA



- Molecule 1: Acetyltransferase ypeA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.05Å 134.39Å 70.47Å 90.00° 105.93° 90.00°	Depositor
Resolution (Å)	34.62 – 2.00 34.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (34.62-2.00) 94.2 (34.62-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.193 , 0.266 0.221 , 0.287	Depositor DCC
R_{free} test set	7359 reflections (9.53%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10253	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, ZN, EDO

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	0.93	0/1225	1.01	1/1640 (0.1%)
1	B	0.87	0/1248	0.98	1/1675 (0.1%)
1	C	0.86	1/1199 (0.1%)	1.05	1/1605 (0.1%)
1	D	0.97	0/1231	1.04	1/1649 (0.1%)
1	E	0.89	0/1183	0.98	1/1586 (0.1%)
1	F	0.90	1/1219 (0.1%)	1.01	2/1632 (0.1%)
1	G	0.91	0/1234	1.02	3/1652 (0.2%)
1	H	0.95	1/1217 (0.1%)	1.06	2/1631 (0.1%)
All	All	0.91	3/9756 (0.0%)	1.02	12/13070 (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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	VAL	CA-CB	6.96	1.63	1.54
1	F	107	VAL	CA-CB	5.69	1.61	1.54
1	H	103	ILE	CA-C	5.64	1.59	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	139	GLU	N-CA-C	7.57	122.63	111.96
1	F	29	ASP	CA-C-N	5.62	125.15	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	29	ASP	C-N-CA	5.62	125.15	119.19
1	B	37	LYS	N-CA-C	-5.61	105.25	111.36
1	H	53	GLU	CA-C-N	-5.44	115.57	122.37
1	H	53	GLU	C-N-CA	-5.44	115.57	122.37
1	A	79	ARG	N-CA-C	5.39	119.85	113.28
1	G	75	HIS	CA-C-N	5.30	125.36	119.32
1	G	75	HIS	C-N-CA	5.30	125.36	119.32
1	G	54	VAL	N-CA-CB	5.25	116.26	110.53
1	D	58	VAL	N-CA-C	-5.08	101.64	108.35
1	C	90	ARG	N-CA-C	-5.01	106.33	112.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1209	0	1156	26	0
1	B	1229	0	1172	40	0
1	C	1183	0	1146	28	0
1	D	1215	0	1174	43	0
1	E	1167	0	1128	42	0
1	F	1203	0	1164	45	0
1	G	1218	0	1175	32	0
1	H	1201	0	1155	28	0
2	B	2	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	B	4	0	3	10	0
3	H	4	0	3	0	0
4	D	4	0	6	5	0
4	E	4	0	6	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	12	0	18	7	0
4	H	8	0	12	2	0
5	A	76	0	0	10	0
5	B	73	0	0	6	0
5	C	64	0	0	1	0
5	D	73	0	0	8	0
5	E	66	0	0	1	0
5	F	74	0	0	3	0
5	G	67	0	0	4	0
5	H	94	0	0	4	0
All	All	10253	0	9318	267	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 14.

All (267) 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:A:55:VAL:HG23	5:A:191:HOH:O	1.39	1.21
1:D:120:ARG:HG2	5:F:670:HOH:O	1.47	1.13
1:H:34:ILE:HG22	1:H:38:MSE:HE2	1.27	1.12
1:E:34:ILE:HG22	1:E:38:MSE:HE2	1.33	1.10
1:D:34:ILE:HG22	1:D:38:MSE:HE2	1.28	1.08
1:B:34:ILE:HG22	1:B:38:MSE:HE2	1.38	1.06
1:F:34:ILE:HG22	1:F:38:MSE:HE2	1.08	1.06
1:D:35:GLU:HA	1:D:38:MSE:HE3	1.35	1.03
1:F:29:ASP:CB	1:F:32:MSE:HE2	1.87	1.03
1:C:34:ILE:HG22	1:C:38:MSE:HE2	1.03	1.02
1:F:29:ASP:HB3	1:F:32:MSE:HE2	1.02	1.02
1:B:62:TYR:H	3:B:607:ACY:H2	1.19	1.02
1:B:1:MSE:HB3	1:B:50:VAL:HG22	1.43	1.00
1:C:35:GLU:HA	1:C:38:MSE:HE3	1.43	0.99
1:F:29:ASP:HB3	1:F:32:MSE:CE	1.92	0.97
1:A:104:GLN:NE2	5:A:208:HOH:O	2.01	0.92
1:F:44:LEU:HD12	4:F:609:EDO:H11	1.48	0.92
1:B:1:MSE:HB3	1:B:50:VAL:CG2	1.99	0.92
1:F:44:LEU:HD12	4:F:609:EDO:C1	2.00	0.91
1:H:111[A]:ASN:H	1:H:111[A]:ASN:HD22	1.14	0.90
1:A:102:LYS:HZ2	1:B:27[A]:TRP:HZ3	0.96	0.89
1:B:62:TYR:N	3:B:607:ACY:H2	1.87	0.88
1:F:34:ILE:CG2	1:F:38:MSE:HE2	1.99	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:ILE:HG22	1:G:38:MSE:HE2	1.54	0.88
1:C:34:ILE:CG2	1:C:38:MSE:HE2	1.99	0.85
1:C:19:GLU:HG2	1:C:24:LEU:CD2	2.07	0.84
1:E:35:GLU:HA	1:E:38:MSE:HE3	1.61	0.82
1:E:134:ARG:HH21	4:E:614:EDO:H21	1.44	0.81
1:F:107:VAL:CG2	1:F:115:LEU:HD13	2.10	0.81
1:H:117:MSE:HE2	4:H:613:EDO:H21	1.61	0.81
1:D:81[B]:ARG:HB2	4:D:608:EDO:O2	1.80	0.80
1:F:20[B]:ARG:HG3	1:F:20[B]:ARG:HH11	1.47	0.79
1:A:109[B]:GLU:OE1	5:A:216:HOH:O	2.01	0.78
1:E:115:LEU:HD11	1:F:129:LEU:HD12	1.65	0.78
1:B:102:LYS:HE2	1:B:104:GLN:HE21	1.48	0.77
5:G:668:HOH:O	4:H:611:EDO:H11	1.84	0.77
1:F:107:VAL:HG21	1:F:115:LEU:HD13	1.66	0.76
1:H:111[A]:ASN:HD22	1:H:111[A]:ASN:N	1.81	0.75
1:D:12[B]:GLU:HG3	1:D:13:GLU:OE1	1.87	0.74
1:E:29:ASP:HB3	1:E:32:MSE:HB2	1.67	0.74
1:F:35:GLU:HA	1:F:38:MSE:HE3	1.70	0.73
1:D:124:GLU:OE2	5:D:678:HOH:O	2.05	0.73
1:C:19:GLU:HG2	1:C:24:LEU:HD22	1.69	0.72
1:E:50:VAL:HG13	1:E:51:ASN:HD22	1.54	0.72
1:A:102:LYS:NZ	1:B:27[A]:TRP:HZ3	1.83	0.72
1:H:102:LYS:HE3	5:H:701:HOH:O	1.88	0.72
1:H:117:MSE:HG2	1:H:120:ARG:NH1	2.05	0.72
1:B:62:TYR:O	3:B:607:ACY:H2	1.88	0.72
1:E:27:TRP:CD1	4:E:614:EDO:H22	2.25	0.72
1:C:75:HIS:CE1	1:C:77[B]:GLU:HG2	2.26	0.70
1:C:34:ILE:HG22	1:C:38:MSE:CE	2.00	0.69
1:G:116:GLY:O	1:G:120[B]:ARG:HD3	1.91	0.69
1:D:34:ILE:HG22	1:D:38:MSE:CE	2.14	0.69
1:A:47:VAL:HG12	1:A:57:THR:HG22	1.75	0.67
1:D:79:ARG:HA	4:D:608:EDO:H22	1.76	0.67
1:F:61:GLY:HA2	4:F:609:EDO:H11	1.74	0.67
1:G:88:LEU:HD23	1:G:117:MSE:HE1	1.77	0.67
1:E:74:VAL:O	1:E:79:ARG:NH1	2.28	0.66
1:E:101:PRO:O	1:F:134:ARG:HD3	1.96	0.66
1:F:102:LYS:NZ	1:F:104:GLN:HE21	1.94	0.66
1:H:104:GLN:NE2	5:H:653:HOH:O	2.27	0.66
1:C:75:HIS:ND1	1:C:77[B]:GLU:HG2	2.11	0.66
1:C:28:ASN:ND2	1:C:134:ARG:HH12	1.94	0.65
1:A:55:VAL:CG2	5:A:191:HOH:O	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:VAL:HG23	1:F:79:ARG:HG3	1.79	0.65
1:F:28:ASN:ND2	1:F:134:ARG:HH12	1.95	0.64
1:B:15:ILE:HD11	1:B:34:ILE:HD12	1.80	0.64
3:B:607:ACY:OXT	5:B:609:HOH:O	2.14	0.63
1:C:134:ARG:HD2	1:C:136:ILE:O	1.99	0.63
1:A:75:HIS:HD2	1:A:77:GLU:HB2	1.63	0.62
1:A:75:HIS:CD2	1:A:77:GLU:HB2	2.35	0.61
3:B:607:ACY:H3	5:B:615:HOH:O	1.99	0.61
1:C:15:ILE:HG12	1:C:30:PRO:HB2	1.81	0.61
1:H:34:ILE:HG22	1:H:38:MSE:CE	2.18	0.61
1:D:89[B]:ASN:ND2	5:D:650:HOH:O	2.32	0.61
1:D:133:LYS:NZ	5:D:676:HOH:O	2.32	0.61
1:H:134:ARG:HD2	1:H:136:ILE:O	2.01	0.61
1:B:62:TYR:H	3:B:607:ACY:CH3	2.07	0.61
1:F:75:HIS:CD2	1:F:77:GLU:HB2	2.36	0.61
1:C:19:GLU:HG2	1:C:24:LEU:HD21	1.83	0.60
1:D:35:GLU:CA	1:D:38:MSE:HE3	2.22	0.60
1:C:15:ILE:O	1:C:19:GLU:HG3	2.02	0.60
1:D:27:TRP:HB2	5:D:679:HOH:O	2.02	0.60
1:B:62:TYR:O	3:B:607:ACY:CH3	2.50	0.59
1:G:47:VAL:HG12	1:G:57:THR:HG22	1.84	0.59
1:H:35:GLU:HA	1:H:38:MSE:HE3	1.83	0.59
1:A:13:GLU:OE2	5:A:184:HOH:O	2.17	0.59
1:A:75:HIS:CD2	1:A:77:GLU:H	2.21	0.59
1:G:124[A]:GLU:HG3	1:G:125:HIS:N	2.18	0.59
1:D:26:PRO:O	1:D:140:GLU:HA	2.03	0.58
1:D:35:GLU:HA	1:D:38:MSE:CE	2.21	0.58
1:B:17:LEU:HD23	1:B:57:THR:HG23	1.85	0.58
1:B:34:ILE:O	1:B:38:MSE:HG3	2.04	0.58
5:A:205:HOH:O	1:H:120:ARG:HD3	2.04	0.57
1:D:72:LEU:CD2	1:D:88:LEU:CD2	2.81	0.57
1:G:60:GLY:HA3	1:G:91:LEU:HD11	1.85	0.57
1:D:75:HIS:CE1	1:D:77:GLU:HB2	2.40	0.57
1:F:32:MSE:CE	1:F:138:ASP:CG	2.78	0.57
1:E:38:MSE:HA	1:E:42:VAL:HG13	1.87	0.57
1:G:34:ILE:O	1:G:38:MSE:HG3	2.05	0.57
1:H:7:ARG:NE	1:H:9[A]:GLU:OE2	2.33	0.56
1:F:29:ASP:CB	1:F:32:MSE:CE	2.67	0.56
1:H:77:GLU:HG3	5:H:674:HOH:O	2.06	0.56
1:C:35:GLU:CA	1:C:38:MSE:HE3	2.26	0.55
1:F:74:VAL:CG2	1:F:79:ARG:HG3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:GLU:HA	1:G:38:MSE:HE3	1.88	0.55
1:C:85:ASN:O	1:C:89:ASN:HB2	2.05	0.55
1:G:11:PHE:HE1	1:G:38:MSE:HE2	1.71	0.55
4:F:612:EDO:H11	5:F:686:HOH:O	2.06	0.55
1:E:11:PHE:HE1	1:E:38:MSE:HE1	1.72	0.54
1:E:50:VAL:CG1	1:E:51:ASN:HD22	2.19	0.54
1:D:34:ILE:C	1:D:38:MSE:HE2	2.33	0.54
1:G:124[A]:GLU:CG	1:G:125:HIS:N	2.70	0.54
1:G:9:GLU:O	5:G:661:HOH:O	2.18	0.54
1:F:20[B]:ARG:HG3	1:F:20[B]:ARG:NH1	2.20	0.54
1:F:32:MSE:HE3	1:F:138:ASP:CG	2.33	0.54
1:H:111[A]:ASN:H	1:H:111[A]:ASN:ND2	1.92	0.54
1:B:9[B]:GLU:CD	1:B:9[B]:GLU:H	2.15	0.54
1:D:72:LEU:HD22	1:D:88:LEU:CD2	2.38	0.53
1:A:53[A]:GLU:HG2	1:A:55:VAL:HG13	1.90	0.53
1:C:18:TRP:HB3	1:C:24:LEU:HD13	1.90	0.53
1:D:38:MSE:HA	1:D:42:VAL:HG13	1.89	0.53
1:E:4:ARG:HB2	1:G:8:GLN:HE21	1.72	0.53
1:F:107:VAL:HG22	1:F:115:LEU:HD13	1.88	0.53
1:A:32:MSE:HG3	1:D:93:LYS:HG3	1.90	0.53
1:F:11:PHE:CD1	1:F:34:ILE:HG21	2.43	0.53
1:C:46:LEU:HD21	1:C:94:LYS:HE3	1.90	0.53
1:F:53:GLU:HB2	5:F:667:HOH:O	2.08	0.52
1:G:15:ILE:O	1:G:19[B]:GLU:HG3	2.09	0.52
1:B:35:GLU:CD	1:B:38:MSE:HE3	2.34	0.52
1:A:12[B]:GLU:HB2	5:A:158:HOH:O	2.10	0.52
1:E:12:GLU:H	1:E:12:GLU:CD	2.16	0.52
1:G:101:PRO:O	1:H:134:ARG:HD3	2.10	0.52
1:D:74:VAL:HG11	4:D:608:EDO:H21	1.92	0.52
1:F:32:MSE:HE1	1:F:138:ASP:CB	2.40	0.52
1:E:111:ASN:HB3	1:E:114:VAL:HG13	1.92	0.51
1:G:38:MSE:HA	1:G:42:VAL:HG13	1.92	0.51
1:B:51:ASN:OD1	1:B:51:ASN:O	2.29	0.51
1:B:111[B]:ASN:CG	1:B:114:VAL:HG12	2.35	0.51
1:E:50:VAL:O	1:E:51:ASN:HB2	2.10	0.51
1:C:75:HIS:HB3	1:C:78:PHE:HD2	1.76	0.51
1:F:32:MSE:HE1	1:F:138:ASP:HB3	1.94	0.50
1:F:102:LYS:HZ1	1:F:104:GLN:HE21	1.59	0.50
1:C:56:GLY:HA2	1:C:73:GLY:O	2.11	0.50
1:D:74:VAL:HG11	4:D:608:EDO:C2	2.41	0.50
1:D:15:ILE:O	1:D:19[A]:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:VAL:HG12	1:F:57:THR:HG22	1.94	0.50
1:G:9:GLU:HG2	5:G:618:HOH:O	2.11	0.50
1:G:26:PRO:HD2	1:G:27:TRP:CZ3	2.47	0.50
1:G:131:LEU:HD21	1:H:115:LEU:HD23	1.93	0.50
1:A:83:ILE:HD13	5:A:191:HOH:O	2.11	0.50
1:B:22[A]:ASP:OD2	5:B:638:HOH:O	2.20	0.50
1:B:34:ILE:CG2	1:B:38:MSE:HE2	2.26	0.50
1:C:134:ARG:HD3	1:D:101:PRO:O	2.12	0.50
1:C:18:TRP:CD1	1:C:23:LEU:HD12	2.48	0.49
1:E:11:PHE:HE1	1:E:38:MSE:CE	2.25	0.49
1:H:108:PRO:HB2	1:H:111[A]:ASN:ND2	2.28	0.49
1:B:35:GLU:OE1	1:B:38:MSE:HE3	2.11	0.49
1:E:49:GLU:HA	1:E:53:GLU:O	2.11	0.49
5:C:152:HOH:O	1:D:65:HIS:HD2	1.95	0.49
1:H:1:MSE:HG2	1:H:50:VAL:HG22	1.94	0.49
1:F:85[A]:ASN:OD1	1:F:85[A]:ASN:C	2.56	0.49
1:F:56:GLY:HA2	1:F:73:GLY:O	2.13	0.49
1:C:129:LEU:HD12	1:D:115:LEU:HD11	1.95	0.49
1:D:26:PRO:HG2	5:D:680:HOH:O	2.13	0.49
1:G:11:PHE:CE1	1:G:38:MSE:HE2	2.47	0.49
1:E:29:ASP:CB	1:E:32:MSE:HB2	2.40	0.48
1:A:11:PHE:CD1	1:A:34:ILE:HG21	2.49	0.48
1:B:85:ASN:HD21	1:B:121:LEU:HD21	1.78	0.48
1:E:11:PHE:CE1	1:E:38:MSE:HE1	2.49	0.48
1:D:12[A]:GLU:CD	1:D:12[A]:GLU:H	2.22	0.47
1:F:32:MSE:HE1	1:F:138:ASP:CG	2.39	0.47
1:E:38:MSE:HA	1:E:42:VAL:CG1	2.44	0.47
1:B:62:TYR:CA	3:B:607:ACY:H2	2.45	0.47
1:E:4:ARG:HB2	1:G:8:GLN:NE2	2.30	0.47
1:D:118:TYR:O	1:D:123:TYR:HB2	2.15	0.47
1:F:75:HIS:HD2	1:F:77:GLU:HB2	1.79	0.47
1:B:13:GLU:HG2	5:B:619:HOH:O	2.15	0.47
1:F:1:MSE:HE2	1:F:1:MSE:HB3	1.91	0.47
1:H:75:HIS:HD1	1:H:77:GLU:H	1.63	0.47
1:D:83:ILE:HB	4:D:608:EDO:H21	1.96	0.47
1:D:111:ASN:C	1:D:111:ASN:HD22	2.22	0.47
1:C:46:LEU:CD2	1:C:94:LYS:HE3	2.44	0.46
1:B:1:MSE:HB3	1:B:50:VAL:HG23	1.89	0.46
1:F:44:LEU:HD12	4:F:609:EDO:C2	2.45	0.46
1:E:129:LEU:HD12	1:F:115:LEU:HD21	1.98	0.46
1:D:139:GLU:HB3	1:D:141:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASP:CG	4:F:609:EDO:H22	2.40	0.46
1:A:54:VAL:HG12	5:A:172:HOH:O	2.16	0.46
1:B:27[A]:TRP:O	1:B:138:ASP:HB2	2.16	0.46
3:B:607:ACY:CH3	5:B:615:HOH:O	2.59	0.46
1:G:88:LEU:CD2	1:G:117:MSE:HE1	2.44	0.46
1:C:131:LEU:HD11	1:D:115:LEU:HD23	1.97	0.46
1:E:76:PRO:HA	1:E:79:ARG:HG2	1.98	0.46
1:B:20:ARG:HD3	1:B:75:HIS:NE2	2.32	0.45
1:B:27[A]:TRP:CZ2	1:B:134:ARG:HD3	2.51	0.45
1:H:72:LEU:HD22	1:H:88:LEU:HD13	1.97	0.45
1:C:118:TYR:HA	1:C:121:LEU:HD12	1.99	0.45
1:D:72:LEU:HD21	1:D:88:LEU:CD2	2.46	0.45
1:H:35:GLU:OE1	1:H:38:MSE:HE3	2.17	0.45
1:H:88:LEU:HD21	1:H:118:TYR:CE1	2.50	0.45
1:B:20:ARG:HA	5:B:647:HOH:O	2.16	0.45
1:D:88:LEU:HD13	1:D:88:LEU:HA	1.82	0.45
1:H:89:ASN:ND2	5:H:645:HOH:O	2.50	0.45
1:E:92:GLU:OE1	1:F:133:LYS:NZ	2.43	0.45
1:E:94:LYS:NZ	1:G:35:GLU:OE1	2.49	0.45
1:A:66:ARG:HB2	1:B:70:TYR:OH	2.17	0.45
1:D:26:PRO:HD2	5:D:680:HOH:O	2.17	0.45
1:H:13[B]:GLU:OE1	1:H:54:VAL:HG13	2.17	0.45
1:D:12[B]:GLU:HG3	1:D:13:GLU:CD	2.41	0.45
1:A:107:VAL:HG13	1:B:131:LEU:HD22	1.99	0.44
1:E:136:ILE:HB	1:F:101:PRO:HA	1.99	0.44
1:G:11:PHE:CE1	1:G:38:MSE:CE	3.00	0.44
1:B:38:MSE:HA	1:B:42:VAL:HG13	1.98	0.44
1:G:11:PHE:HE1	1:G:38:MSE:CE	2.31	0.44
1:H:74:VAL:O	1:H:75:HIS:C	2.56	0.44
1:B:1:MSE:HE1	1:B:86:ALA:CB	2.47	0.43
1:B:31:GLU:O	1:B:35:GLU:HG2	2.18	0.43
1:F:41:ASP:OD2	4:F:609:EDO:H22	2.18	0.43
1:E:11:PHE:HE2	1:E:31:GLU:HG2	1.83	0.43
1:E:47:VAL:HG12	1:E:57:THR:HG22	2.00	0.43
1:A:19:GLU:HG2	1:A:24:LEU:CD1	2.49	0.43
1:A:105:ILE:HD12	1:A:123:TYR:CE1	2.53	0.43
1:E:7:ARG:O	1:E:8:GLN:C	2.62	0.43
1:E:35:GLU:OE1	1:E:38:MSE:HE3	2.18	0.43
1:E:29:ASP:HB3	1:E:32:MSE:CB	2.44	0.43
1:G:11:PHE:CD1	1:G:34:ILE:HG21	2.54	0.42
1:H:113:MSE:O	1:H:117:MSE:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:HD22	1:C:134:ARG:HH12	1.66	0.42
1:F:134:ARG:HD2	1:F:136:ILE:O	2.19	0.42
1:D:32:MSE:HG2	1:D:36:ARG:CZ	2.49	0.42
1:F:32:MSE:HE2	1:F:32:MSE:HB2	1.66	0.42
1:F:102:LYS:HZ3	1:F:104:GLN:HE21	1.65	0.42
1:G:28:ASN:ND2	1:G:134:ARG:HH22	2.18	0.42
1:E:75:HIS:HD2	1:E:77:GLU:H	1.67	0.42
1:B:3:ILE:HG12	1:B:87:LEU:HD13	2.01	0.42
1:D:27:TRP:N	5:D:679:HOH:O	2.07	0.42
1:A:25:ARG:CZ	5:A:205:HOH:O	2.67	0.42
1:E:5:VAL:H	1:G:8:GLN:NE2	2.18	0.42
1:E:118:TYR:HB3	1:F:131:LEU:HD23	2.02	0.42
1:G:65:HIS:HA	5:G:605:HOH:O	2.19	0.42
1:B:88:LEU:HD23	1:B:117:MSE:CE	2.50	0.41
1:E:28:ASN:O	1:E:30:PRO:HD3	2.19	0.41
1:H:47:VAL:HG12	1:H:57:THR:HG22	2.02	0.41
1:A:107:VAL:CG1	1:B:131:LEU:HD22	2.50	0.41
1:E:50:VAL:O	1:E:53:GLU:HG2	2.21	0.41
1:C:18:TRP:HB3	1:C:24:LEU:CD1	2.49	0.41
1:E:46:LEU:HB2	1:E:58:VAL:HG12	2.02	0.41
1:D:95:LEU:HB3	1:D:100:CYS:HB3	2.03	0.41
1:E:134:ARG:HH21	4:E:614:EDO:C2	2.24	0.41
1:G:110[A]:ASP:O	1:G:112:ASP:OD1	2.38	0.41
1:B:50:VAL:O	1:B:51:ASN:HB3	2.21	0.41
1:D:19[A]:GLU:HG2	1:D:24:LEU:HD11	2.02	0.41
1:E:76:PRO:HA	1:E:79:ARG:CG	2.51	0.41
1:A:65:HIS:O	1:A:66:ARG:HD3	2.21	0.41
1:B:62:TYR:C	3:B:607:ACY:H2	2.46	0.41
1:E:51:ASN:N	5:E:665:HOH:O	2.53	0.41
1:C:13[A]:GLU:CD	1:C:13[A]:GLU:H	2.29	0.40
1:B:25:ARG:HD3	1:B:27[B]:TRP:CZ2	2.56	0.40
1:D:133:LYS:HZ2	1:D:133:LYS:HG2	1.50	0.40
1:A:19:GLU:CG	1:A:24:LEU:HD11	2.51	0.40
1:E:5:VAL:H	1:G:8:GLN:HE22	1.69	0.40
1:A:60:GLY:HA3	1:A:91:LEU:CD1	2.51	0.40
1:D:41:ASP:HA	5:D:671:HOH:O	2.20	0.40
1:H:50:VAL:HG23	1:H:55:VAL:HG21	2.04	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	147/144 (102%)	142 (97%)	4 (3%)	1 (1%)	18	14
1	B	148/144 (103%)	140 (95%)	8 (5%)	0	100	100
1	C	144/144 (100%)	139 (96%)	3 (2%)	2 (1%)	9	4
1	D	147/144 (102%)	140 (95%)	6 (4%)	1 (1%)	18	14
1	E	142/144 (99%)	132 (93%)	8 (6%)	2 (1%)	9	4
1	F	146/144 (101%)	136 (93%)	8 (6%)	2 (1%)	9	4
1	G	147/144 (102%)	137 (93%)	7 (5%)	3 (2%)	6	2
1	H	146/144 (101%)	140 (96%)	5 (3%)	1 (1%)	18	14
All	All	1167/1152 (101%)	1106 (95%)	49 (4%)	12 (1%)	12	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	41	ASP
1	D	41	ASP
1	G	41	ASP
1	A	41	ASP
1	E	41	ASP
1	F	41	ASP
1	F	139	GLU
1	C	1	MSE
1	E	111	ASN
1	G	19[A]	GLU
1	G	19[B]	GLU
1	H	41	ASP

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	129/118 (109%)	121 (94%)	8 (6%)	16	13
1	B	131/118 (111%)	123 (94%)	8 (6%)	17	14
1	C	126/118 (107%)	114 (90%)	12 (10%)	8	5
1	D	129/118 (109%)	123 (95%)	6 (5%)	23	22
1	E	125/118 (106%)	113 (90%)	12 (10%)	8	5
1	F	128/118 (108%)	117 (91%)	11 (9%)	10	6
1	G	130/118 (110%)	118 (91%)	12 (9%)	8	5
1	H	129/118 (109%)	118 (92%)	11 (8%)	10	7
All	All	1027/944 (109%)	947 (92%)	80 (8%)	14	8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2[A]	GLU
1	A	2[B]	GLU
1	A	49	GLU
1	A	89	ASN
1	A	107	VAL
1	A	128	VAL
1	A	137[A]	GLU
1	A	137[B]	GLU
1	B	19[A]	GLU
1	B	19[B]	GLU
1	B	85	ASN
1	B	87	LEU
1	B	88	LEU
1	B	107	VAL
1	B	115	LEU
1	B	120	ARG
1	C	2[A]	GLU
1	C	2[B]	GLU
1	C	8	GLN
1	C	13[A]	GLU
1	C	13[B]	GLU
1	C	24	LEU
1	C	51	ASN

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Mol	Chain	Res	Type
1	C	74	VAL
1	C	81	ARG
1	C	89	ASN
1	C	107	VAL
1	C	115	LEU
1	D	8	GLN
1	D	88	LEU
1	D	93	LYS
1	D	110	ASP
1	D	131	LEU
1	D	141	TYR
1	E	12	GLU
1	E	32	MSE
1	E	50	VAL
1	E	79	ARG
1	E	88	LEU
1	E	109	GLU
1	E	110[A]	ASP
1	E	110[B]	ASP
1	E	114	VAL
1	E	115	LEU
1	E	139	GLU
1	E	140	GLU
1	F	1	MSE
1	F	2	GLU
1	F	3	ILE
1	F	13[A]	GLU
1	F	13[B]	GLU
1	F	20[A]	ARG
1	F	20[B]	ARG
1	F	32	MSE
1	F	107	VAL
1	F	113	MSE
1	F	115	LEU
1	G	1	MSE
1	G	2	GLU
1	G	77[A]	GLU
1	G	77[B]	GLU
1	G	112	ASP
1	G	115	LEU
1	G	117	MSE
1	G	119[A]	GLU

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Mol	Chain	Res	Type
1	G	119[B]	GLU
1	G	120[A]	ARG
1	G	120[B]	ARG
1	G	131	LEU
1	H	1	MSE
1	H	7	ARG
1	H	19	GLU
1	H	53	GLU
1	H	54	VAL
1	H	110[A]	ASP
1	H	110[B]	ASP
1	H	111[A]	ASN
1	H	111[B]	ASN
1	H	113	MSE
1	H	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	75	HIS
1	A	111	ASN
1	B	51	ASN
1	B	85	ASN
1	B	104	GLN
1	B	106	ASN
1	C	28	ASN
1	C	51	ASN
1	D	65	HIS
1	D	85	ASN
1	D	111	ASN
1	E	51	ASN
1	E	75	HIS
1	E	111	ASN
1	F	28	ASN
1	F	89	ASN
1	F	104	GLN
1	G	8	GLN
1	G	28	ASN
1	H	89	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\# Z > 2$
3	ACY	H	606	-	3,3,3	0.90	0	3,3,3	0.79	0
4	EDO	D	608	-	3,3,3	0.38	0	2,2,2	0.64	0
4	EDO	E	614	-	3,3,3	0.45	0	2,2,2	0.54	0
4	EDO	F	610	-	3,3,3	0.59	0	2,2,2	0.33	0
4	EDO	H	611	-	3,3,3	0.41	0	2,2,2	0.66	0
3	ACY	B	607	-	3,3,3	1.91	2 (66%)	3,3,3	1.55	1 (33%)
4	EDO	H	613	-	3,3,3	0.43	0	2,2,2	0.86	0
4	EDO	F	612	-	3,3,3	0.58	0	2,2,2	0.34	0
4	EDO	F	609	-	3,3,3	0.49	0	2,2,2	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	608	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	614	-	-	0/1/1/1	-
4	EDO	F	610	-	-	0/1/1/1	-
4	EDO	H	611	-	-	1/1/1/1	-
4	EDO	H	613	-	-	0/1/1/1	-
4	EDO	F	612	-	-	0/1/1/1	-
4	EDO	F	609	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	607	ACY	O-C	-2.35	1.12	1.22
3	B	607	ACY	OXT-C	-2.26	1.20	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	607	ACY	OXT-C-CH3	2.01	123.48	115.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	611	EDO	O1-C1-C2-O2
4	D	608	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	608	EDO	5	0
4	E	614	EDO	3	0
4	H	611	EDO	1	0
3	B	607	ACY	10	0
4	H	613	EDO	1	0
4	F	612	EDO	1	0
4	F	609	EDO	6	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, 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	134/144 (93%)	0.32	4 (2%)	52	51	16, 30, 41, 51	8 (5%)
1	B	135/144 (93%)	0.44	4 (2%)	52	51	13, 31, 45, 53	9 (6%)
1	C	134/144 (93%)	0.49	4 (2%)	52	51	15, 32, 46, 55	6 (4%)
1	D	136/144 (94%)	0.30	3 (2%)	62	61	11, 30, 46, 57	7 (5%)
1	E	134/144 (93%)	0.45	5 (3%)	45	44	15, 31, 45, 49	4 (2%)
1	F	135/144 (93%)	0.33	3 (2%)	62	61	13, 31, 43, 55	7 (5%)
1	G	132/144 (91%)	0.37	4 (3%)	52	51	13, 30, 39, 43	11 (8%)
1	H	134/144 (93%)	0.36	1 (0%)	84	84	15, 32, 42, 50	8 (5%)
All	All	1074/1152 (93%)	0.38	28 (2%)	57	56	11, 31, 44, 57	60 (5%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27[A]	TRP	5.3
1	C	0	ALA	3.9
1	E	50	VAL	3.6
1	D	0	ALA	3.4
1	E	75	HIS	3.0
1	D	141	TYR	3.0
1	H	51	ASN	2.9
1	C	80	GLY	2.8
1	F	80	GLY	2.7
1	A	80	GLY	2.6
1	E	52	GLY	2.6
1	E	112	ASP	2.6
1	A	20	ARG	2.4
1	A	110	ASP	2.3
1	G	9	GLU	2.3
1	A	0	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	55	VAL	2.3
1	D	26	PRO	2.3
1	E	51	ASN	2.3
1	G	51	ASN	2.2
1	C	2[A]	GLU	2.2
1	G	80	GLY	2.2
1	B	75	HIS	2.1
1	F	0	ALA	2.1
1	G	120[A]	ARG	2.1
1	C	76	PRO	2.0
1	B	50	VAL	2.0
1	B	112	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
4	EDO	H	611	4/4	0.76	0.21	41,43,43,43	0
4	EDO	H	613	4/4	0.76	0.16	41,42,42,46	0
4	EDO	E	614	4/4	0.78	0.20	49,52,54,58	0
4	EDO	F	612	4/4	0.80	0.13	41,46,46,47	0
4	EDO	F	610	4/4	0.82	0.11	43,45,47,47	0
4	EDO	D	608	4/4	0.90	0.13	19,28,34,38	0
3	ACY	B	607	4/4	0.90	0.16	23,25,28,29	0
3	ACY	H	606	4/4	0.91	0.10	39,39,39,40	0
4	EDO	F	609	4/4	0.92	0.17	11,19,22,25	0
2	ZN	B	604	1/1	0.94	0.07	48,48,48,48	1
2	ZN	H	605	1/1	0.98	0.03	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	601	1/1	0.98	0.04	34,34,34,34	1
2	ZN	E	602	1/1	0.99	0.04	30,30,30,30	1
2	ZN	G	603	1/1	0.99	0.02	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.