



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:31 PM GMT

PDB ID : 5AB0  
Title : Crystal structure of aminopeptidase ERAP2 with ligand  
Authors : Mpakali, A.; Giastas, P.; Saridakis, E.; Stratikos, E.  
Deposited on : 2015-07-31  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

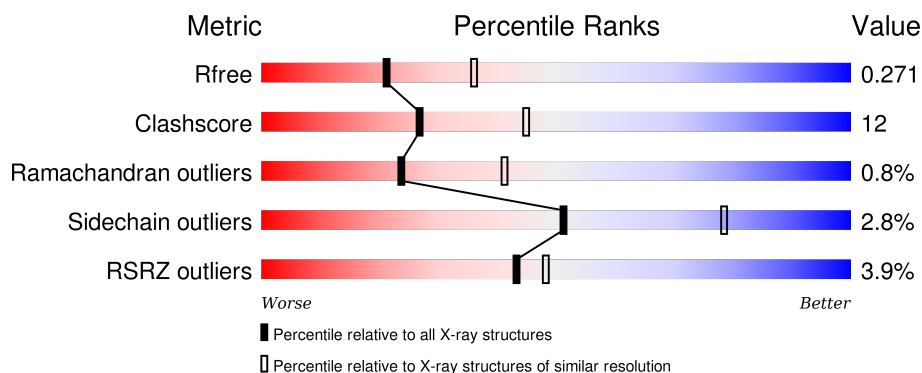
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	967	<div> <div></div> <div>72% 21% • 6%</div> </div>
1	C	967	<div> <div>6%</div> <div>61% 29% • 9%</div> </div>
2	E	10	<div> <div>10% 60% 30%</div> </div>
2	F	10	<div> <div>40% 40% 50% 10%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15615 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 ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	911	Total	C	N	O	S	0	4	1
			7425	4779	1236	1378	32			
1	C	882	Total	C	N	O	S	0	4	1
			7208	4646	1196	1338	28			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ARG	-	EXPRESSION TAG	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
A	392	ASN	LYS	VARIANT	UNP Q6P179
C	961	ARG	-	EXPRESSION TAG	UNP Q6P179
C	962	HIS	-	EXPRESSION TAG	UNP Q6P179
C	963	HIS	-	EXPRESSION TAG	UNP Q6P179
C	964	HIS	-	EXPRESSION TAG	UNP Q6P179
C	965	HIS	-	EXPRESSION TAG	UNP Q6P179
C	966	HIS	-	EXPRESSION TAG	UNP Q6P179
C	967	HIS	-	EXPRESSION TAG	UNP Q6P179
C	392	ASN	LYS	VARIANT	UNP Q6P179

- Molecule 2 is a protein called DG025.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			
2	F	10	Total	C	N	O	P	0	0	0
			93	64	16	12	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

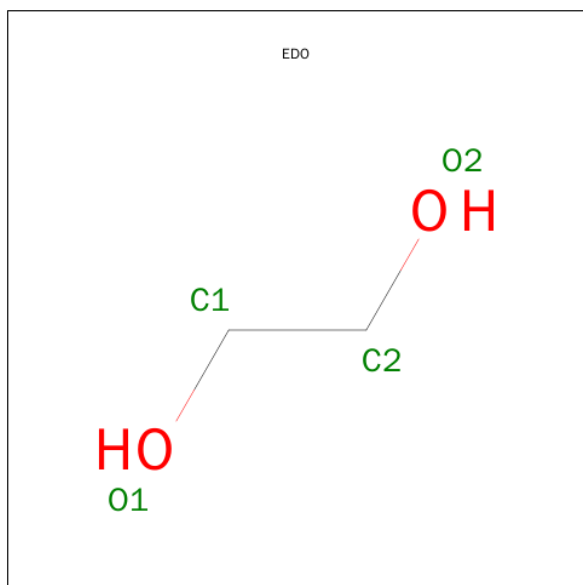
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

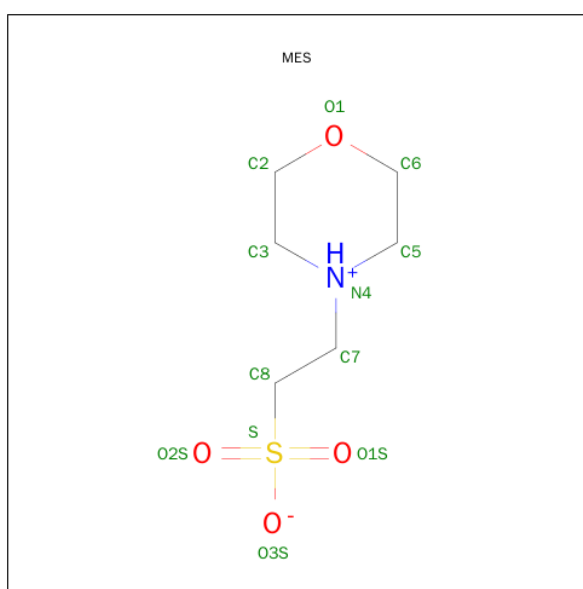
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	278	Total	O	0	0
			278	278		

Continued on next page...

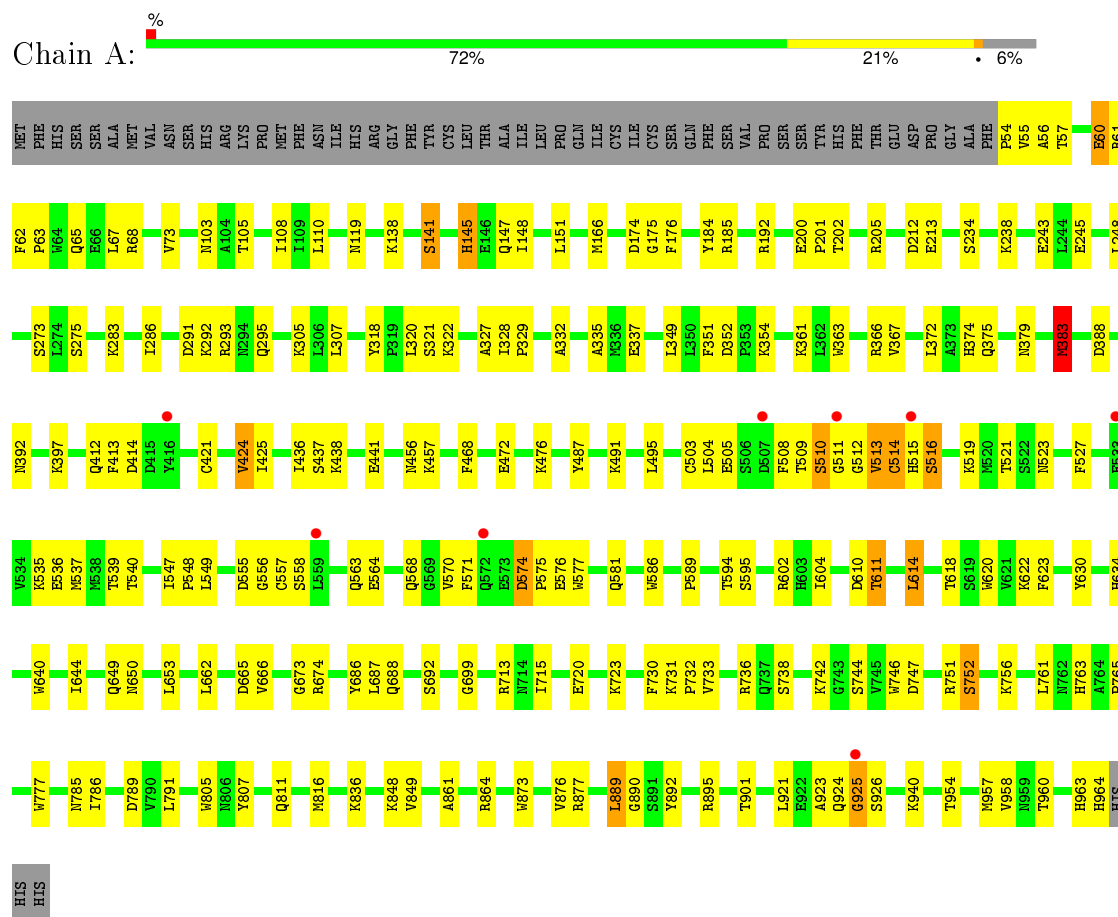
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	125	Total 125	O 125	0	0

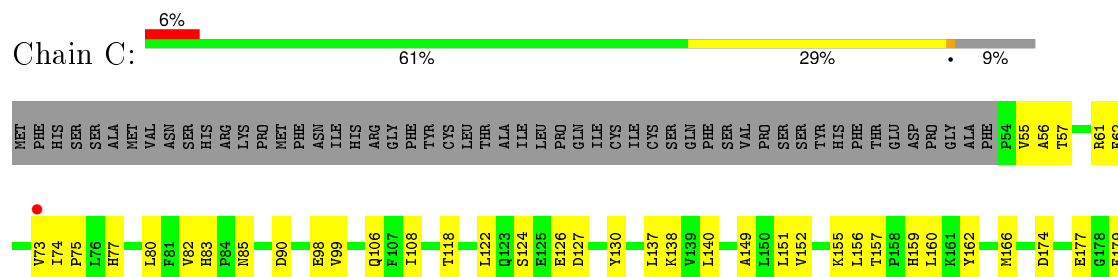
### 3 Residue-property plots

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.

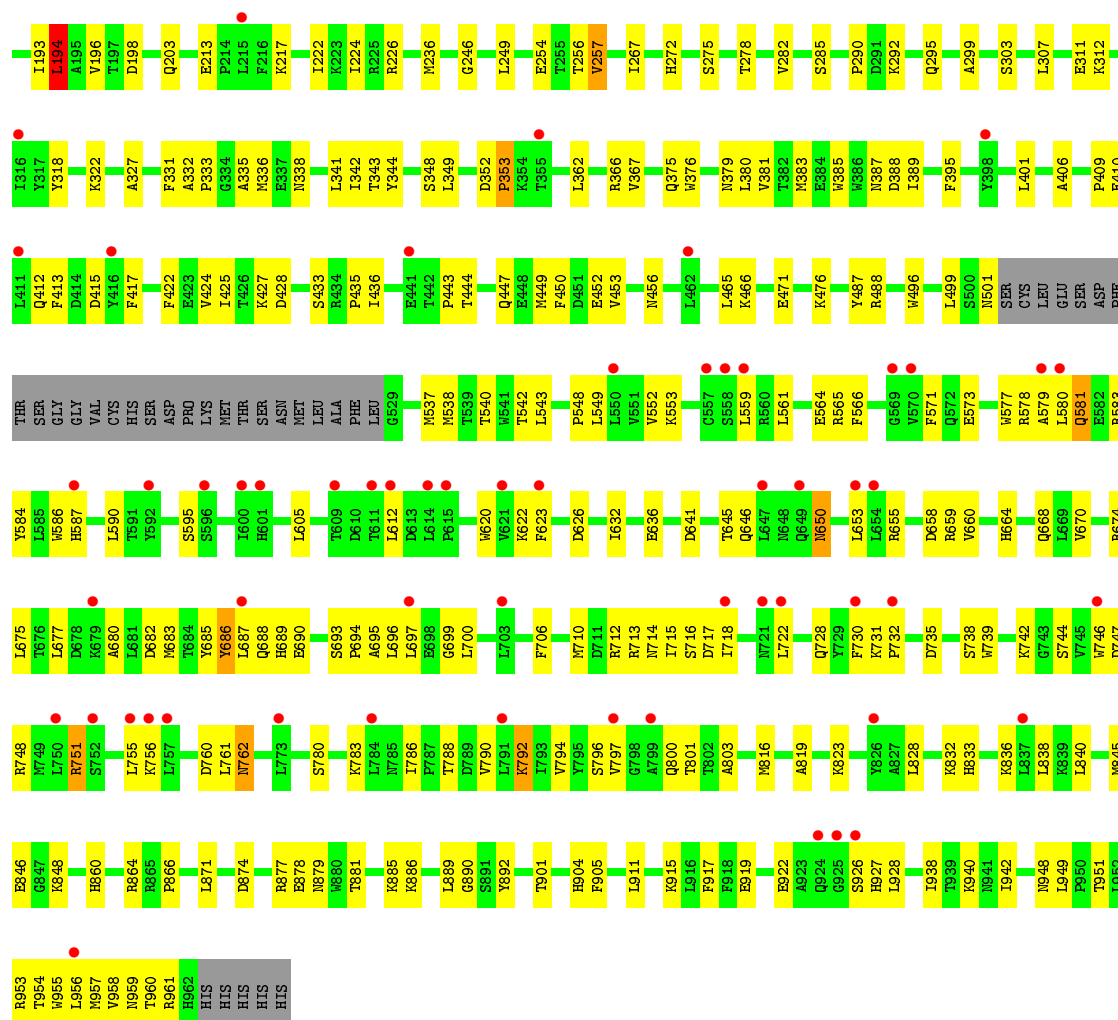
#### • Molecule 1: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2




#### • Molecule 1: ENDOPLASMATIC RETICULUM AMINOPEPTIDASE 2







● Molecule 2: DG025

Chain E: 



● Molecule 2: DG025

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.35Å 134.42Å 129.00Å 90.00° 90.49° 90.00°	Depositor
Resolution (Å)	65.73 – 2.50 67.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.73-2.50) 93.7 (67.21-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.198 , 0.258 0.216 , 0.271	Depositor DCC
$R_{free}$ test set	4421 reflections (5.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.7	EDS
Estimated twinning fraction	0.016 for -h,-l,-k 0.002 for -h,l,k 0.029 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 88270 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, 7GA, NAG, EDO, MES, 2X0, LYN

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	0/7620	0.62	1/10327 (0.0%)
1	C	0.41	0/7395	0.57	1/10021 (0.0%)
2	E	0.73	0/65	0.85	0/85
2	F	0.39	0/65	0.65	0/85
All	All	0.46	0/15145	0.60	2/20518 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	383	MET	CG-SD-CE	-5.80	90.91	100.20
1	C	194	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	889	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7425	0	7350	149	0
1	C	7208	0	7148	198	0
2	E	93	0	91	14	0
2	F	93	0	92	12	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	56	0	52	1	0
4	C	84	0	78	0	0
5	A	56	0	50	0	0
5	C	28	0	25	0	0
6	A	78	0	68	1	0
7	A	8	0	12	3	0
7	C	8	0	12	1	0
8	A	12	0	12	0	0
9	C	61	0	52	3	0
10	A	278	0	0	28	0
10	C	125	0	0	23	0
All	All	15615	0	15042	366	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 12.

All (366) 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:C:922:GLU:HA	1:C:926:SER:HB3	1.46	0.97
1:C:424:VAL:HG22	1:C:452:GLU:HB3	1.50	0.94
1:C:424:VAL:HG21	1:C:456:ASN:HB2	1.48	0.93
1:A:720:GLU:OE2	10:A:3217:HOH:O	1.86	0.93
1:A:508:PHE:H	1:A:509:THR:HA	1.36	0.88
1:C:55:VAL:HG13	1:C:62:PHE:HB2	1.56	0.87
1:C:106:GLN:HG2	1:C:155:LYS:HG2	1.58	0.85
1:A:472:GLU:OE1	10:A:3159:HOH:O	1.95	0.83
1:C:717:ASP:OD2	1:C:953:ARG:NH1	2.12	0.82
1:A:291:ASP:OD1	10:A:3095:HOH:O	1.95	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:PHE:N	1:A:509:THR:HA	1.92	0.80
1:A:595:SER:HG	1:A:618:THR:HG1	1.29	0.80
1:A:964:HIS:N	10:A:3268:HOH:O	2.14	0.79
1:A:213:GLU:OE1	10:A:3006:HOH:O	2.01	0.78
1:C:157:THR:HB	1:C:160:LEU:HD12	1.65	0.77
1:C:138:LYS:HD2	1:C:151:LEU:HD12	1.65	0.77
1:A:563:GLN:OE1	10:A:3178:HOH:O	2.02	0.77
1:C:174:ASP:OD2	10:C:3027:HOH:O	2.01	0.75
1:A:61:ARG:NH1	10:A:3001:HOH:O	2.20	0.74
1:C:488:ARG:O	10:C:3043:HOH:O	2.04	0.74
2:E:6:ALA:HA	2:E:8:SER:N	2.03	0.73
1:C:838:LEU:HG	1:C:871:LEU:HD21	1.71	0.72
1:C:659:ARG:NH1	1:C:690:GLU:OE2	2.22	0.72
1:A:576:GLU:OE2	10:A:3183:HOH:O	2.07	0.72
1:A:662:LEU:O	1:A:666:VAL:HG23	1.89	0.72
1:C:587:HIS:ND1	10:C:3084:HOH:O	2.23	0.71
1:C:83:HIS:NE2	9:C:1003:NAG:H81	2.04	0.71
1:C:911:LEU:HD13	1:C:938:ILE:HB	1.72	0.70
1:C:162:TYR:O	10:C:3014:HOH:O	2.09	0.70
1:C:919:GLU:O	10:C:3112:HOH:O	2.10	0.69
1:C:90:ASP:OD2	10:C:3011:HOH:O	2.10	0.69
1:C:56:ALA:HB1	1:C:57:THR:HA	1.73	0.69
1:A:367:VAL:HG13	2:E:2:7GA:H102	1.74	0.69
1:C:951:THR:OG1	10:C:3115:HOH:O	2.10	0.69
2:E:3:LYS:C	2:E:5:HIS:H	1.96	0.68
2:F:3:LYS:O	2:F:5:HIS:N	2.19	0.68
1:C:198:ASP:OD2	10:C:3034:HOH:O	2.11	0.67
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.75	0.67
1:C:85:ASN:HD22	9:C:1003:NAG:H83	1.58	0.67
1:A:438:LYS:NZ	10:A:3148:HOH:O	2.15	0.66
1:A:564:GLU:OE1	1:A:674:ARG:NH2	2.29	0.66
1:C:465:LEU:HB2	1:C:538:MET:HE3	1.76	0.66
2:E:3:LYS:O	2:E:5:HIS:N	2.27	0.66
2:F:1:2X0:C17	2:F:3:LYS:HG2	2.25	0.66
1:C:381:VAL:HA	10:C:3043:HOH:O	1.96	0.66
1:C:845:MET:O	1:C:886:LYS:NZ	2.30	0.65
1:A:594:THR:HB	1:A:618:THR:HG21	1.78	0.65
1:C:713:ARG:CD	1:C:715:ILE:HD11	2.26	0.65
1:C:677:LEU:HD22	1:C:948:ASN:HB3	1.79	0.65
1:A:895:ARG:NE	10:A:3255:HOH:O	2.29	0.64
1:A:504:LEU:HD23	1:A:505:GLU:H	1.61	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:PHE:HB3	1:A:512:GLY:HA3	1.78	0.64
1:C:140:LEU:HB2	1:C:149:ALA:HB3	1.78	0.64
1:C:713:ARG:HD2	1:C:715:ILE:HD11	1.80	0.63
1:C:257:VAL:HG11	1:C:487:TYR:CE1	2.33	0.63
1:A:293:ARG:NH2	9:C:1001:BMA:O2	2.28	0.63
1:A:414:ASP:OD2	10:A:3141:HOH:O	2.15	0.63
1:A:723:LYS:HG3	1:A:761:LEU:HB3	1.81	0.63
1:C:940:LYS:NZ	10:C:3114:HOH:O	2.30	0.63
1:A:521:THR:HG22	1:A:523:ASN:H	1.64	0.63
2:E:6:ALA:HA	2:E:7:PHE:C	2.19	0.63
1:A:55:VAL:HG22	1:A:62:PHE:H	1.62	0.62
2:F:1:2X0:H11	2:F:3:LYS:HG2	1.81	0.62
1:C:549:LEU:HB2	1:C:566:PHE:HB2	1.81	0.62
1:A:424:VAL:HG11	1:A:457:LYS:HB2	1.82	0.61
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.82	0.61
1:C:55:VAL:CG2	1:C:62:PHE:H	2.13	0.61
1:C:213:GLU:HG2	1:C:385:TRP:HZ3	1.66	0.61
1:C:122:LEU:HB2	1:C:137:LEU:HD11	1.81	0.61
1:A:513:VAL:HG11	1:A:527:PHE:CD2	2.35	0.61
1:C:622:LYS:NZ	1:C:658:ASP:OD1	2.34	0.61
1:A:892:TYR:CD1	2:E:3:LYS:HD3	2.35	0.61
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.83	0.60
1:A:713:ARG:NE	10:A:3213:HOH:O	2.21	0.60
1:A:602:ARG:NH1	10:A:3186:HOH:O	2.24	0.60
1:A:185:ARG:HD3	10:A:3042:HOH:O	2.01	0.59
1:C:55:VAL:HG21	1:C:61:ARG:HA	1.85	0.59
1:C:874:ASP:O	1:C:878:GLU:HB2	2.02	0.59
1:C:118:THR:OG1	10:C:3019:HOH:O	2.16	0.59
1:C:55:VAL:HG21	1:C:62:PHE:H	1.66	0.58
1:C:786:ILE:HD13	1:C:794:VAL:HG11	1.85	0.58
1:C:650:ASN:HD22	1:C:653:LEU:HD21	1.68	0.58
1:C:682:ASP:OD1	1:C:955:TRP:NE1	2.28	0.58
1:C:452:GLU:OE2	10:C:3081:HOH:O	2.16	0.58
1:C:77:HIS:HB3	1:C:98:GLU:HB3	1.86	0.58
1:A:283:LYS:NZ	7:A:1965:EDO:H12	2.19	0.58
1:A:692:SER:OG	10:A:3197:HOH:O	2.17	0.57
1:C:670:VAL:O	10:C:3093:HOH:O	2.17	0.57
1:C:646:GLN:HE22	1:C:653:LEU:HD12	1.69	0.57
2:E:1:2X0:H11	2:E:3:LYS:HB3	1.86	0.57
1:C:196:VAL:HG13	1:C:267:ILE:HG12	1.86	0.57
1:C:716:SER:HB3	10:C:3096:HOH:O	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLU:OE1	1:A:576:GLU:N	2.31	0.57
1:C:443:PRO:O	1:C:447:GLN:HG3	2.05	0.57
1:C:792:LYS:HE3	1:C:823:LYS:HD2	1.88	0.56
1:A:555:ASP:HB2	1:A:558:SER:HB3	1.87	0.56
1:A:923:ALA:N	1:A:924:GLN:O	2.38	0.56
1:C:626:ASP:OD2	1:C:655:ARG:NH1	2.39	0.56
1:C:877:ARG:HG3	1:C:917:PHE:CD1	2.42	0.55
1:C:687:LEU:HD11	1:C:699:GLY:HA3	1.87	0.55
1:A:513:VAL:HG11	1:A:527:PHE:CG	2.42	0.55
1:C:688:GLN:OE1	1:C:689:HIS:N	2.39	0.55
1:C:450:PHE:O	2:F:3:LYS:HE3	2.07	0.55
1:A:54:PRO:HB2	10:A:3001:HOH:O	2.05	0.55
1:C:236:MET:HG2	1:C:256:THR:HG22	1.87	0.55
1:A:61:ARG:HH22	1:A:65:GLN:HE21	1.53	0.55
1:A:640:TRP:O	1:A:644:ILE:HG13	2.05	0.55
2:E:5:HIS:O	2:E:7:PHE:HB3	2.06	0.55
1:C:177:GLU:HG2	1:C:203:GLN:HG2	1.88	0.54
1:C:595:SER:HB3	1:C:620:TRP:H	1.70	0.54
1:C:641:ASP:O	1:C:645:THR:OG1	2.17	0.54
1:C:738:SER:O	1:C:751:ARG:HD3	2.08	0.54
4:A:1069:NAG:O4	10:A:3269:HOH:O	2.15	0.54
1:A:508:PHE:HB2	1:A:514:CYS:O	2.08	0.54
1:A:892:TYR:CG	2:E:3:LYS:HD3	2.43	0.54
1:C:80:LEU:HD23	1:C:222:ILE:HD12	1.90	0.54
1:A:436:ILE:HD11	1:A:457:LYS:HG2	1.89	0.54
1:A:67:LEU:HD21	1:A:441:GLU:HB3	1.89	0.54
1:A:57:THR:HG23	1:A:141:SER:O	2.08	0.54
1:A:412:GLN:HG3	1:A:746:TRP:CD1	2.43	0.54
1:C:780:SER:HB2	1:C:783:LYS:HB2	1.90	0.54
1:C:685:TYR:OH	1:C:959:ASN:ND2	2.38	0.54
1:C:389:ILE:HG21	1:C:449:MET:HB3	1.90	0.53
1:C:424:VAL:CG2	1:C:456:ASN:HB2	2.32	0.53
1:A:184:TYR:CE1	1:A:192:ARG:HB2	2.43	0.53
1:C:756:LYS:NZ	1:C:760:ASP:OD2	2.41	0.53
1:C:864:ARG:HH12	2:F:9:PHE:HB2	1.73	0.53
1:C:366:ARG:NH2	10:C:3067:HOH:O	2.40	0.53
1:C:564:GLU:OE2	1:C:674:ARG:NH2	2.41	0.53
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.44	0.53
1:C:680:ALA:O	1:C:683:MET:HB3	2.08	0.53
1:C:718:ILE:HD13	1:C:949:LEU:HD11	1.89	0.53
1:C:954:THR:O	1:C:958:VAL:HG23	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1077:NAG:HO3	6:A:1078:BMA:HO2	1.57	0.53
1:A:650:ASN:HB3	1:A:653:LEU:HG	1.92	0.52
1:A:805:TRP:CD2	1:A:836:LYS:HD2	2.44	0.52
1:C:292:LYS:HE2	1:C:816:MET:O	2.09	0.52
1:A:491:LYS:HD2	10:A:3166:HOH:O	2.09	0.52
1:C:801:THR:HG22	1:C:803:ALA:H	1.74	0.52
1:C:580:LEU:H	1:C:583:ARG:HE	1.57	0.52
1:C:226:ARG:HH12	1:C:249:LEU:HD12	1.74	0.52
1:C:780:SER:O	1:C:783:LYS:HG2	2.10	0.52
1:C:697:LEU:HD23	1:C:700:LEU:HD12	1.92	0.52
1:C:922:GLU:HA	1:C:926:SER:CB	2.30	0.51
1:C:659:ARG:HB3	1:C:686:TYR:OH	2.10	0.51
1:A:335:ALA:O	2:E:2:7GA:H62C	2.11	0.51
1:C:713:ARG:HD3	1:C:715:ILE:HD11	1.91	0.51
1:A:508:PHE:N	1:A:509:THR:CA	2.69	0.51
1:C:573:GLU:N	1:C:573:GLU:OE1	2.29	0.51
1:A:924:GLN:O	1:A:926:SER:N	2.39	0.51
1:A:200:GLU:OE2	10:A:3052:HOH:O	2.17	0.51
1:C:664:HIS:O	1:C:668:GLN:HG2	2.11	0.51
1:C:761:LEU:O	1:C:762:ASN:HB2	2.11	0.51
1:C:311:GLU:OE2	1:C:318:TYR:N	2.42	0.50
1:C:905:PHE:O	1:C:938:ILE:HG23	2.12	0.50
1:C:126:GLU:HB3	1:C:160:LEU:HD22	1.93	0.50
2:F:1:2X0:H11	2:F:3:LYS:HB3	1.94	0.50
1:A:924:GLN:HG2	1:A:925:GLY:N	2.26	0.50
1:A:571:PHE:HD1	1:A:673:GLY:HA3	1.73	0.50
1:C:436:ILE:HG22	1:C:453:VAL:HG13	1.92	0.50
1:C:595:SER:HA	1:C:620:TRP:CE2	2.47	0.50
1:C:332:ALA:HB3	1:C:333:PRO:HD3	1.93	0.50
1:A:889:LEU:N	1:A:890:GLY:HA3	2.26	0.50
1:C:819:ALA:O	1:C:823:LYS:HG2	2.12	0.49
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.94	0.49
1:A:742:LYS:O	1:A:751:ARG:NH2	2.44	0.49
1:A:777:TRP:HH2	1:A:811:GLN:HG3	1.77	0.49
1:A:337:GLU:HG3	1:A:374:HIS:HB3	1.95	0.49
1:C:590:LEU:HD11	1:C:605:LEU:HB2	1.94	0.49
1:C:55:VAL:HG12	1:C:56:ALA:O	2.11	0.49
1:C:487:TYR:HA	10:C:3041:HOH:O	2.12	0.49
1:C:792:LYS:O	1:C:796:SER:OG	2.18	0.49
1:A:861:ALA:HA	1:A:864:ARG:HE	1.78	0.49
1:C:213:GLU:HG2	1:C:385:TRP:CZ3	2.48	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLN:HG2	1:A:940:LYS:HZ3	1.78	0.49
1:C:646:GLN:NE2	1:C:653:LEU:HD12	2.28	0.49
1:A:571:PHE:CD1	1:A:673:GLY:HA3	2.47	0.49
1:A:738:SER:O	1:A:751:ARG:HD3	2.12	0.49
1:A:807:TYR:O	1:A:811:GLN:HG2	2.12	0.49
1:C:748:ARG:NH2	1:C:788:THR:OG1	2.46	0.49
1:A:505:GLU:HG3	1:A:508:PHE:O	2.12	0.48
1:C:226:ARG:NH1	1:C:249:LEU:HD12	2.28	0.48
1:C:537:MET:O	1:C:540:THR:OG1	2.24	0.48
1:A:201:PRO:HB2	1:A:202:THR:HG23	1.95	0.48
1:C:344:TYR:CD1	1:C:349:LEU:HD13	2.48	0.48
1:A:273:SER:HA	1:A:286:ILE:O	2.13	0.48
1:A:921:LEU:O	1:A:926:SER:HB2	2.14	0.48
1:C:427:LYS:O	1:C:433:SER:OG	2.32	0.48
1:A:610:ASP:OD1	1:A:611:THR:N	2.44	0.48
1:C:98:GLU:HG3	10:C:3014:HOH:O	2.13	0.48
1:A:848:LYS:N	10:A:3246:HOH:O	2.40	0.48
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.49	0.48
1:C:236:MET:HB3	1:C:254:GLU:HB3	1.96	0.48
1:A:73:VAL:HG21	1:A:108:ILE:HG23	1.95	0.48
1:C:278:THR:HG21	1:C:307:LEU:HD23	1.96	0.48
1:A:375:GLN:O	1:A:379:ASN:HB2	2.14	0.48
1:A:568:GLN:HG2	1:A:940:LYS:NZ	2.29	0.47
1:C:742:LYS:O	1:C:751:ARG:NH2	2.47	0.47
1:C:889:LEU:HG	1:C:928:LEU:HD21	1.96	0.47
1:C:138:LYS:HB2	1:C:138:LYS:HE3	1.54	0.47
1:A:640:TRP:CZ3	1:A:666:VAL:HG22	2.50	0.47
1:A:425:ILE:HG12	1:A:547:ILE:HD13	1.95	0.47
1:C:435:PRO:HA	10:C:3075:HOH:O	2.14	0.47
1:C:922:GLU:HB2	10:C:3112:HOH:O	2.14	0.47
1:C:376:TRP:HA	1:C:380:LEU:HB3	1.96	0.47
1:C:739:TRP:CE3	1:C:790:VAL:HG11	2.49	0.47
1:A:574:ASP:OD1	1:A:575:PRO:HD2	2.15	0.47
2:E:1:2X0:C18	2:E:3:LYS:HG2	2.45	0.46
2:F:3:LYS:C	2:F:5:HIS:N	2.68	0.46
1:A:547:ILE:HD12	1:A:630:TYR:CD2	2.49	0.46
1:C:406:ALA:N	10:C:3073:HOH:O	2.22	0.46
1:A:665:ASP:OD2	10:A:3199:HOH:O	2.21	0.46
1:C:217:LYS:NZ	10:C:3041:HOH:O	2.34	0.46
1:C:548:PRO:HB3	1:C:586:TRP:CE3	2.50	0.46
1:A:383:MET:HE3	1:A:392:ASN:OD1	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ASN:O	1:C:716:SER:N	2.48	0.46
1:C:412:GLN:CD	1:C:746:TRP:HD1	2.19	0.46
1:C:731:LYS:N	1:C:732:PRO:HD2	2.31	0.46
1:C:577:TRP:CE3	1:C:578:ARG:HB2	2.51	0.46
1:C:127:ASP:HB2	1:C:160:LEU:HD13	1.98	0.46
2:E:3:LYS:C	2:E:5:HIS:N	2.63	0.46
1:C:832:LYS:HE3	1:C:833:HIS:NE2	2.31	0.46
1:C:838:LEU:HD21	1:C:871:LEU:HD11	1.98	0.46
1:A:924:GLN:HG2	1:A:925:GLY:H	1.81	0.46
1:A:622:LYS:NZ	1:A:623:PHE:O	2.39	0.46
1:C:348:SER:HB2	1:C:367:VAL:HG21	1.98	0.46
1:C:338:ASN:HB2	1:C:341:LEU:O	2.16	0.46
1:A:849:VAL:N	10:A:3246:HOH:O	2.47	0.45
1:A:366:ARG:HD2	1:A:413:PHE:CZ	2.51	0.45
1:A:876:VAL:HG21	1:A:901:THR:HG21	1.98	0.45
1:A:275:SER:O	10:A:3085:HOH:O	2.20	0.45
1:C:466:LYS:HE3	1:C:471[B]:GLU:HG3	1.98	0.45
1:A:510:SER:HA	1:A:511:GLY:HA2	1.55	0.45
1:C:559:LEU:HD11	1:C:612:LEU:HB2	1.97	0.45
1:A:549:LEU:HD11	1:A:634:HIS:HB2	1.99	0.45
1:C:422:PHE:HA	1:C:425:ILE:HD12	1.98	0.45
1:C:55:VAL:HG12	1:C:56:ALA:N	2.32	0.45
1:A:283:LYS:HZ3	7:A:1965:EDO:H12	1.81	0.45
1:A:731:LYS:N	1:A:732:PRO:HD2	2.32	0.45
1:A:570:VAL:HG12	1:A:577:TRP:HD1	1.81	0.45
1:A:744:SER:N	1:A:747:ASP:OD2	2.41	0.45
1:C:675:LEU:O	10:C:3092:HOH:O	2.21	0.45
1:A:777:TRP:CH2	1:A:811:GLN:HG3	2.52	0.45
1:C:375:GLN:O	1:C:379:ASN:HB2	2.17	0.45
1:C:73:VAL:HG11	1:C:108:ILE:HG23	1.99	0.45
1:A:110:LEU:HD11	1:A:148:ILE:HD11	1.98	0.45
2:F:3:LYS:C	2:F:5:HIS:H	2.12	0.45
1:A:176:PHE:CG	1:A:332:ALA:HB2	2.52	0.45
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.52	0.45
1:C:878:GLU:HB3	1:C:879:ASN:ND2	2.32	0.44
1:C:82:VAL:HB	1:C:224:ILE:HD13	1.99	0.44
1:A:756:LYS:HE3	2:E:10:LYN:HG2	1.99	0.44
1:A:752:SER:HB3	1:A:789:ASP:O	2.18	0.44
1:C:846:GLU:HG3	1:C:848:LYS:H	1.81	0.44
1:C:650:ASN:HB3	1:C:653:LEU:HG	1.98	0.44
1:C:410:GLU:H	1:C:410:GLU:CD	2.20	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LYS:O	1:A:539:THR:HG23	2.18	0.44
1:A:732:PRO:HB2	1:A:736:ARG:HH21	1.82	0.44
1:A:354:LYS:HE3	1:A:785:ASN:OD1	2.17	0.44
1:A:67:LEU:HD12	1:A:68:ARG:N	2.33	0.44
1:C:577:TRP:HZ3	1:C:578:ARG:HD3	1.82	0.44
1:A:62:PHE:HA	1:A:63:PRO:HD3	1.84	0.44
1:A:424:VAL:HG22	1:A:456:ASN:CB	2.48	0.44
1:A:56:ALA:HB1	1:A:57:THR:HA	1.99	0.44
1:C:124:SER:HB2	1:C:130:TYR:HB2	1.98	0.44
1:C:336:MET:O	1:C:342:ILE:HG23	2.18	0.44
1:A:318:TYR:CE2	1:A:320:LEU:HB2	2.53	0.44
1:C:670:VAL:HG21	1:C:680:ALA:HB2	2.00	0.43
1:A:292:LYS:HE2	1:A:816:MET:O	2.18	0.43
1:A:145:HIS:O	1:A:147:GLN:HG3	2.18	0.43
1:A:363:TRP:O	1:A:367:VAL:HG23	2.18	0.43
1:A:957:MET:O	1:A:960:THR:HB	2.18	0.43
1:C:901:THR:HA	1:C:904:HIS:HE1	1.83	0.43
1:C:696:LEU:O	1:C:700:LEU:HG	2.18	0.43
1:A:119:ASN:O	1:A:166:MET:HA	2.19	0.43
1:C:295:GLN:HG2	1:C:352:ASP:HB2	2.00	0.43
1:A:397:LYS:HE2	10:A:3153:HOH:O	2.17	0.43
1:A:328:ILE:HA	1:A:329:PRO:HD3	1.81	0.43
1:A:205:ARG:HH21	1:A:212:ASP:HB3	1.83	0.43
1:C:415:ASP:HB3	1:C:694:PRO:HG3	2.01	0.43
1:C:246:GLY:N	10:C:3053:HOH:O	2.52	0.43
1:C:739:TRP:CZ2	1:C:755:LEU:HD22	2.54	0.43
1:C:797:VAL:O	1:C:800:GLN:HG2	2.19	0.43
1:C:553:LYS:HB2	1:C:636:GLU:OE1	2.19	0.43
1:C:892:TYR:HB2	2:F:3:LYS:HD2	2.00	0.43
1:A:514:CYS:HA	1:A:515:HIS:HA	1.77	0.43
1:C:282:VAL:HG22	7:C:1962:EDO:H11	2.01	0.43
1:A:516:SER:O	10:A:3172:HOH:O	2.21	0.43
1:A:307:LEU:HD13	1:A:372:LEU:HD13	2.00	0.42
1:C:74:ILE:HA	1:C:75:PRO:HD2	1.90	0.42
1:C:889:LEU:N	1:C:890:GLY:HA3	2.34	0.42
1:C:476:LYS:NZ	1:C:501:ASN:O	2.50	0.42
1:C:299:ALA:O	1:C:303:SER:HB2	2.19	0.42
1:C:331:PHE:HZ	1:C:343:THR:HG1	1.64	0.42
1:A:476:LYS:HG2	1:A:503:CYS:O	2.19	0.42
1:A:954:THR:O	1:A:958:VAL:HG23	2.20	0.42
1:A:595:SER:HB3	1:A:620:TRP:CE2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:HB2	1:C:349:LEU:HD23	2.01	0.42
1:C:706:PHE:O	1:C:710:MET:HG2	2.19	0.42
1:C:722:LEU:HG	1:C:956:LEU:HD21	2.00	0.42
2:E:1:2X0:H12	2:E:3:LYS:HG2	2.00	0.42
1:A:55:VAL:HG13	1:A:60:GLU:O	2.20	0.42
1:A:487:TYR:HA	10:A:3060:HOH:O	2.20	0.42
1:C:362:LEU:HD11	1:C:413:PHE:CD1	2.54	0.42
1:C:836:LYS:HA	1:C:836:LYS:HD3	1.73	0.42
1:A:549:LEU:N	1:A:564:GLU:O	2.46	0.42
1:C:786:ILE:HG21	1:C:794:VAL:HG21	2.01	0.42
1:A:468:PHE:CZ	1:A:604:ILE:HD11	2.54	0.42
1:C:387:ASN:OD1	1:C:388:ASP:N	2.53	0.42
1:C:660:VAL:HG22	1:C:695:ALA:HA	2.01	0.42
1:C:881:THR:O	1:C:885:LYS:HG3	2.20	0.42
1:A:537:MET:HE2	1:A:589:PRO:HD3	2.02	0.42
1:C:312:LYS:HE3	1:C:312:LYS:HB2	1.87	0.42
1:C:687:LEU:HA	1:C:687:LEU:HD23	1.83	0.42
1:C:193:ILE:CG2	1:C:194:LEU:N	2.83	0.42
1:A:388:ASP:OD1	1:A:437:SER:OG	2.33	0.42
1:C:577:TRP:O	1:C:581:GLN:HB3	2.19	0.42
1:A:295:GLN:HG2	1:A:352:ASP:HB2	2.02	0.42
2:F:1:2X0:H11	2:F:3:LYS:CG	2.50	0.41
1:C:715:ILE:H	1:C:715:ILE:HG13	1.69	0.41
1:C:744:SER:N	1:C:747:ASP:HB2	2.34	0.41
1:C:565:ARG:HD2	1:C:584:TYR:CG	2.55	0.41
1:C:272:HIS:CE1	1:C:290:PRO:HB3	2.54	0.41
1:C:152:VAL:HG11	1:C:156:LEU:HD21	2.02	0.41
1:C:828:LEU:HB3	1:C:840:LEU:HD11	2.03	0.41
1:C:693:SER:N	1:C:694:PRO:HD2	2.35	0.41
1:A:351:PHE:CZ	1:A:361:LYS:HE2	2.54	0.41
1:A:245[A]:GLU:CD	1:A:245[A]:GLU:H	2.24	0.41
1:C:864:ARG:HH22	2:F:9:PHE:HB3	1.85	0.41
1:A:495:LEU:O	1:A:495:LEU:HG	2.20	0.41
1:C:552:VAL:HG22	1:C:561:LEU:CD2	2.51	0.41
1:C:712:ARG:HA	1:C:866:PRO:HG3	2.01	0.41
1:C:938:ILE:O	1:C:942:ILE:HG13	2.20	0.41
1:C:157:THR:O	1:C:160:LEU:HB2	2.21	0.41
1:A:424:VAL:HG22	1:A:456:ASN:HB2	2.03	0.41
1:C:622:LYS:HE2	1:C:623:PHE:O	2.21	0.41
1:C:926:SER:HB2	1:C:927:HIS:HA	2.03	0.41
1:C:401:LEU:HD13	1:C:417:PHE:HB2	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HB3	1:A:238:LYS:HE2	1.82	0.41
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.90	0.41
1:C:731:LYS:HG3	1:C:735:ASP:OD2	2.21	0.41
1:C:542:THR:C	1:C:543:LEU:HD23	2.41	0.41
1:C:496:TRP:HA	1:C:499:LEU:HB2	2.03	0.41
1:C:860:HIS:O	1:C:864:ARG:HD3	2.21	0.41
1:A:175:GLY:O	1:A:176:PHE:HB2	2.20	0.41
1:C:565:ARG:HD2	1:C:584:TYR:CD1	2.55	0.41
1:A:536:GLU:O	1:A:540:THR:HG23	2.21	0.41
1:A:557:CYS:HB2	1:A:614:LEU:O	2.20	0.41
1:A:519:LYS:HD2	1:A:519:LYS:HA	1.81	0.41
1:C:955:TRP:HE3	1:C:956:LEU:HD12	1.85	0.41
1:A:174:ASP:N	1:A:174:ASP:OD1	2.48	0.41
1:C:55:VAL:HG11	1:C:62:PHE:N	2.36	0.40
1:A:805:TRP:CE2	1:A:836:LYS:HD2	2.56	0.40
1:A:577:TRP:O	1:A:581:GLN:HG2	2.21	0.40
1:C:915:LYS:O	1:C:919:GLU:HG2	2.21	0.40
1:C:713:ARG:HD2	1:C:715:ILE:CD1	2.50	0.40
1:A:421:CYS:O	1:A:424:VAL:HG23	2.22	0.40
1:C:352:ASP:HA	1:C:353:PRO:HD3	1.73	0.40
1:C:444:THR:HG23	1:C:890:GLY:HA2	2.04	0.40
1:C:409:PRO:HD2	1:C:410:GLU:OE1	2.22	0.40
1:A:786:ILE:HB	1:A:791:LEU:HD13	2.03	0.40
7:A:1965:EDO:H11	10:A:3119:HOH:O	2.20	0.40
1:A:305:LYS:O	10:A:3106:HOH:O	2.21	0.40
1:C:335:ALA:O	2:F:2:7GA:H62C	2.21	0.40
1:A:248:LEU:HA	1:A:248:LEU:HD23	1.90	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	913/967 (94%)	851 (93%)	56 (6%)	6 (1%)	26	46
1	C	882/967 (91%)	815 (92%)	61 (7%)	6 (1%)	26	46
2	E	7/10 (70%)	3 (43%)	2 (29%)	2 (29%)	0	0
2	F	7/10 (70%)	3 (43%)	3 (43%)	1 (14%)	0	0
All	All	1809/1954 (93%)	1672 (92%)	122 (7%)	15 (1%)	24	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	SER
1	A	516	SER
2	E	4	HIS
2	F	4	HIS
1	A	730	PHE
1	A	925	GLY
1	A	60	GLU
1	C	579	ALA
1	C	581	GLN
1	A	556	GLY
1	C	728	GLN
1	C	730	PHE
2	E	7	PHE
1	C	762	ASN
1	C	353	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	822/870 (94%)	801 (97%)	21 (3%)	54	81
1	C	796/870 (92%)	775 (97%)	21 (3%)	54	81
2	E	6/6 (100%)	4 (67%)	2 (33%)	0	0
2	F	6/6 (100%)	5 (83%)	1 (17%)	3	5
All	All	1630/1752 (93%)	1585 (97%)	45 (3%)	51	78

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	105	THR
1	A	141	SER
1	A	145	HIS
1	A	234	SER
1	A	243	GLU
1	A	321	SER
1	A	322	LYS
1	A	383	MET
1	A	424	VAL
1	A	513	VAL
1	A	514	CYS
1	A	574	ASP
1	A	611	THR
1	A	614	LEU
1	A	649	GLN
1	A	686	TYR
1	A	688	GLN
1	A	733	VAL
1	A	752	SER
1	A	963	HIS
1	C	99	VAL
1	C	159	HIS
1	C	166	MET
1	C	179	PHE
1	C	194	LEU
1	C	257	VAL
1	C	275	SER
1	C	285	SER
1	C	322	LYS
1	C	383	MET
1	C	395	PHE
1	C	428	ASP
1	C	571	PHE
1	C	632	ILE
1	C	650	ASN
1	C	686	TYR
1	C	751	ARG
1	C	792	LYS
1	C	957	MET
1	C	960	THR
1	C	961	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	3	LYS
2	E	8	SER
2	F	3	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LYN	E	10	2	9,9,9	1.82	1 (11%)	8,10,10	1.04	0
2	LYN	F	10	2	9,9,9	1.80	1 (11%)	8,10,10	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYN	E	10	2	-	0/8/9/9	0/0/0/0
2	LYN	F	10	2	-	0/8/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	10	LYN	C-NT	5.28	1.43	1.32

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10	LYN	C-NT	5.34	1.43	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	10	LYN	1	0

## 5.5 Carbohydrates ⓘ

17 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1071	1,5	14,14,15	0.55	0	15,19,21	0.32	0
5	NAG	A	1072	5	14,14,15	0.46	0	15,19,21	0.44	0
6	NAG	A	1073	1,6	14,14,15	0.60	0	15,19,21	0.63	0
6	NAG	A	1074	6	14,14,15	0.66	1 (7%)	15,19,21	0.44	0
6	BMA	A	1075	6	11,11,12	0.77	0	15,15,17	1.34	2 (13%)
6	NAG	A	1076	1,6	14,14,15	0.30	0	15,19,21	1.05	2 (13%)
6	NAG	A	1077	6	14,14,15	1.12	1 (7%)	15,19,21	1.23	1 (6%)
6	BMA	A	1078	6	11,11,12	1.53	2 (18%)	15,15,17	2.18	5 (33%)
5	NAG	A	1079	1,5	14,14,15	1.51	1 (7%)	15,19,21	1.19	2 (13%)
5	NAG	A	1080	5	14,14,15	0.24	0	15,19,21	0.25	0
9	BMA	C	1001	9	11,11,12	2.02	2 (18%)	15,15,17	1.24	2 (13%)
9	BMA	C	1002	9	11,11,12	1.33	2 (18%)	15,15,17	1.40	2 (13%)
9	NAG	C	1003	1,9	14,14,15	0.42	0	15,19,21	0.58	0
9	NAG	C	1004	9	14,14,15	1.12	1 (7%)	15,19,21	1.45	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	BMA	C	1005	9	11,11,12	1.18	1 (9%)	15,15,17	1.22	2 (13%)
5	NAG	C	1007	1,5	14,14,15	0.69	1 (7%)	15,19,21	0.46	0
5	NAG	C	1008	5	14,14,15	0.30	0	15,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1071	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1072	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1073	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1074	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1075	6	-	0/2/19/22	0/1/1/1
6	NAG	A	1076	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1077	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1078	6	-	0/2/19/22	0/1/1/1
5	NAG	A	1079	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1080	5	-	0/6/23/26	0/1/1/1
9	BMA	C	1001	9	-	0/2/19/22	0/1/1/1
9	BMA	C	1002	9	-	0/2/19/22	0/1/1/1
9	NAG	C	1003	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	1004	9	-	0/6/23/26	0/1/1/1
9	BMA	C	1005	9	-	0/2/19/22	0/1/1/1
5	NAG	C	1007	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1008	5	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1079	NAG	O5-C1	-5.37	1.35	1.43
9	C	1001	BMA	C2-C3	-5.16	1.45	1.52
9	C	1004	NAG	O5-C1	-4.13	1.37	1.43
9	C	1001	BMA	C1-C2	-2.97	1.44	1.52
6	A	1074	NAG	O5-C1	-2.35	1.39	1.43
5	C	1007	NAG	O5-C1	-2.24	1.40	1.43
9	C	1002	BMA	C2-C3	-2.22	1.49	1.52
9	C	1002	BMA	C4-C5	2.06	1.57	1.53
9	C	1005	BMA	C2-C3	2.47	1.55	1.52
6	A	1078	BMA	O5-C5	2.88	1.49	1.43
6	A	1078	BMA	C1-C2	3.71	1.61	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1077	NAG	O5-C1	4.02	1.50	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1004	NAG	O4-C4-C3	-3.95	101.46	110.36
6	A	1078	BMA	O2-C2-C3	-3.55	103.04	110.19
9	C	1001	BMA	O2-C2-C3	-3.02	104.09	110.19
6	A	1075	BMA	O2-C2-C3	-2.81	104.52	110.19
9	C	1005	BMA	O2-C2-C3	-2.41	105.34	110.19
6	A	1078	BMA	C3-C4-C5	-2.40	105.94	110.23
5	A	1079	NAG	C1-O5-C5	-2.26	108.81	112.14
9	C	1002	BMA	C1-C2-C3	-2.11	107.00	109.55
6	A	1076	NAG	O4-C4-C3	-2.09	105.64	110.36
9	C	1005	BMA	C1-C2-C3	2.19	112.20	109.55
9	C	1004	NAG	C1-O5-C5	2.52	115.85	112.14
6	A	1076	NAG	C1-O5-C5	2.55	115.88	112.14
5	A	1079	NAG	C3-C4-C5	2.64	114.94	110.23
6	A	1078	BMA	O5-C1-C2	2.72	115.24	110.89
9	C	1001	BMA	C1-O5-C5	2.72	116.14	112.14
6	A	1078	BMA	C1-C2-C3	3.05	113.25	109.55
9	C	1002	BMA	C1-O5-C5	3.52	117.31	112.14
6	A	1075	BMA	C1-O5-C5	3.58	117.40	112.14
6	A	1077	NAG	C1-O5-C5	4.24	118.37	112.14
6	A	1078	BMA	C1-O5-C5	5.57	120.33	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1077	NAG	1	0
6	A	1078	BMA	1	0
9	C	1001	BMA	1	0
9	C	1003	NAG	2	0

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 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$
4	NAG	A	1069	1	14,14,15	0.90	1 (7%)	15,19,21	1.01	1 (6%)
4	NAG	A	1070	1	14,14,15	0.50	0	15,19,21	0.56	0
4	NAG	A	1081	1	14,14,15	0.56	0	15,19,21	0.78	1 (6%)
4	NAG	A	1082	1	14,14,15	0.34	0	15,19,21	0.45	0
7	EDO	A	1964	-	3,3,3	0.54	0	2,2,2	0.26	0
7	EDO	A	1965	-	3,3,3	0.33	0	2,2,2	0.51	0
8	MES	A	2002	-	12,12,12	2.13	1 (8%)	15,16,16	2.51	7 (46%)
4	NAG	C	1006	1	14,14,15	0.67	0	15,19,21	0.61	0
4	NAG	C	1009	1	14,14,15	1.06	2 (14%)	15,19,21	0.82	1 (6%)
4	NAG	C	1010	1	14,14,15	0.20	0	15,19,21	0.40	0
4	NAG	C	1011	1	14,14,15	0.66	1 (7%)	15,19,21	0.56	0
4	NAG	C	1012	1	14,14,15	0.29	0	15,19,21	0.39	0
4	NAG	C	1013	1	14,14,15	0.73	1 (7%)	15,19,21	0.72	1 (6%)
7	EDO	C	1962	-	3,3,3	0.47	0	2,2,2	0.32	0
7	EDO	C	1963	-	3,3,3	0.51	0	2,2,2	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1069	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1070	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1081	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1082	1	-	0/6/23/26	0/1/1/1
7	EDO	A	1964	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1965	-	-	0/1/1/1	0/0/0/0
8	MES	A	2002	-	-	0/6/14/14	0/1/1/1
4	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1012	1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1013	1	-	0/6/23/26	0/1/1/1
7	EDO	C	1962	-	-	0/1/1/1	0/0/0/0
7	EDO	C	1963	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2002	MES	C8-S	-6.98	1.67	1.77
4	C	1009	NAG	O5-C1	-2.88	1.39	1.43
4	C	1011	NAG	O5-C1	-2.31	1.39	1.43
4	C	1013	NAG	C1-C2	2.16	1.55	1.52
4	C	1009	NAG	C1-C2	2.26	1.55	1.52
4	A	1069	NAG	O5-C1	3.08	1.48	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2002	MES	C2-C3-N4	-2.18	106.77	110.11
4	C	1009	NAG	C4-C3-C2	2.16	114.69	111.34
4	C	1013	NAG	C1-O5-C5	2.46	115.76	112.14
8	A	2002	MES	O3S-S-C8	2.60	110.39	104.99
4	A	1081	NAG	C1-O5-C5	2.86	116.35	112.14
8	A	2002	MES	C7-N4-C3	3.35	118.53	111.25
8	A	2002	MES	O1S-S-C8	3.58	109.40	106.87
4	A	1069	NAG	C1-O5-C5	3.59	117.41	112.14
8	A	2002	MES	C7-N4-C5	3.65	119.20	111.25
8	A	2002	MES	C5-N4-C3	4.05	117.93	108.87
8	A	2002	MES	O2S-S-C8	4.25	109.87	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1069	NAG	1	0
7	A	1965	EDO	3	0
7	C	1962	EDO	1	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	911/967 (94%)	0.04	8 (0%) 85 88	22, 44, 77, 103	0
1	C	882/967 (91%)	0.37	59 (6%) 21 23	28, 68, 107, 125	0
2	E	7/10 (70%)	1.05	0 100 100	61, 66, 81, 84	0
2	F	7/10 (70%)	2.52	4 (57%) 0 0	75, 81, 95, 98	0
All	All	1807/1954 (92%)	0.22	71 (3%) 43 48	22, 54, 100, 125	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	580	LEU	5.6
2	F	9	PHE	4.5
2	F	7	PHE	4.5
1	C	746	TRP	4.4
1	C	559	LEU	4.1
1	A	515	HIS	4.1
1	C	647	LEU	4.0
1	C	569	GLY	3.8
1	C	612	LEU	3.6
1	C	956	LEU	3.6
1	C	653	LEU	3.6
1	C	722	LEU	3.6
1	C	687	LEU	3.6
1	C	570	VAL	3.5
1	C	615	PRO	3.3
1	C	614	LEU	3.3
1	A	925	GLY	3.3
1	C	797	VAL	3.3
1	C	592	TYR	3.2
1	C	755	LEU	3.2
1	C	718	ILE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	752	SER	3.1
1	C	654	LEU	3.1
1	C	750	LEU	3.0
1	C	623	PHE	3.0
1	C	721	ASN	2.9
1	C	600	ILE	2.9
2	F	6	ALA	2.9
1	C	601	HIS	2.8
1	C	784	LEU	2.8
1	C	773	LEU	2.7
1	C	697	LEU	2.7
1	A	511	GLY	2.6
1	C	837	LEU	2.6
1	C	732	PRO	2.6
1	C	558	SER	2.6
1	C	215	LEU	2.6
1	A	559	LEU	2.5
1	A	507	ASP	2.5
1	C	411	LEU	2.5
1	C	550	LEU	2.5
1	C	924	GLN	2.5
1	C	596	SER	2.5
1	C	621	VAL	2.4
1	C	462	LEU	2.4
1	C	416	TYR	2.4
1	C	730	PHE	2.4
1	C	579	ALA	2.4
2	F	4	HIS	2.4
1	A	416	TYR	2.4
1	C	799	ALA	2.4
1	C	791	LEU	2.4
1	C	398	TYR	2.3
1	C	441[A]	GLU	2.3
1	C	703	LEU	2.3
1	C	925	GLY	2.3
1	A	533[A]	GLU	2.3
1	C	826	TYR	2.3
1	C	355	THR	2.2
1	C	609	THR	2.2
1	C	557	CYS	2.2
1	C	756	LYS	2.2
1	C	587	HIS	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	679	LYS	2.2
1	C	316	ILE	2.2
1	C	649	GLN	2.1
1	C	926	SER	2.2
1	C	611	THR	2.1
1	A	572	GLN	2.1
1	C	73	VAL	2.0
1	C	757	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	LYN	E	10	10/10	0.62	0.67	-	64,83,107,109	0
2	LYN	F	10	10/10	0.09	0.60	-	87,102,106,122	0

## 6.3 Carbohydrates [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
5	NAG	A	1071	14/15	0.94	0.15	-0.35	44,52,76,76	0
5	NAG	C	1007	14/15	0.91	0.13	-0.56	42,55,65,65	0
9	NAG	C	1003	14/15	0.96	0.13	-0.71	32,38,42,47	0
6	NAG	A	1073	14/15	0.97	0.13	-0.79	33,37,48,55	0
6	NAG	A	1076	14/15	0.93	0.14	-1.13	55,68,81,96	0
5	NAG	A	1072	14/15	0.90	0.15	-	69,82,88,88	0
9	BMA	C	1002	11/12	0.83	0.19	-	81,93,99,100	0
9	BMA	C	1001	11/12	0.89	0.17	-	64,70,84,85	0
6	BMA	A	1078	11/12	0.68	0.20	-	116,118,123,125	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	C	1004	14/15	0.90	0.17	-	35,47,60,62	0
5	NAG	C	1008	14/15	0.83	0.22	-	57,71,82,87	0
9	BMA	C	1005	11/12	0.87	0.12	-	61,69,74,76	0
6	NAG	A	1077	14/15	0.82	0.23	-	87,99,117,117	0
5	NAG	A	1080	14/15	0.69	0.26	-	105,117,121,122	0
6	NAG	A	1074	14/15	0.93	0.13	-	52,61,70,88	0
5	NAG	A	1079	14/15	0.81	0.20	-	89,102,111,118	0
6	BMA	A	1075	11/12	0.80	0.17	-	87,95,100,102	0

## 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	1011	14/15	0.88	0.25	1.23	88,100,105,111	0
4	NAG	C	1009	14/15	0.80	0.20	0.06	87,94,99,104	0
3	ZN	A	1008	1/1	0.99	0.15	-0.88	23,23,23,23	0
7	EDO	C	1962	4/4	0.91	0.12	-1.30	57,61,62,71	0
3	ZN	C	1020	1/1	0.99	0.12	-1.46	39,39,39,39	0
4	NAG	C	1012	14/15	0.62	0.25	-	101,111,116,117	0
4	NAG	A	1081	14/15	0.79	0.18	-	88,103,108,112	0
7	EDO	A	1965	4/4	0.91	0.17	-	56,59,61,74	0
4	NAG	A	1070	14/15	0.90	0.13	-	72,85,96,97	0
4	NAG	A	1082	14/15	0.55	0.33	-	83,98,105,106	0
7	EDO	A	1964	4/4	0.72	0.30	-	57,61,62,62	0
4	NAG	C	1006	14/15	0.74	0.20	-	96,107,113,123	0
4	NAG	A	1069	14/15	0.71	0.21	-	84,98,99,101	0
4	NAG	C	1013	14/15	0.57	0.32	-	108,122,126,127	0
4	NAG	C	1010	14/15	0.78	0.29	-	105,115,120,122	0
7	EDO	C	1963	4/4	0.81	0.20	-	89,91,96,99	0
8	MES	A	2002	12/12	0.78	0.14	-	87,98,123,140	0

## 6.5 Other polymers

There are no such residues in this entry.