



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:23 PM EDT

PDB ID : 7RT7  
Title : Crystal structure of the RhsP2 C-terminal toxin domain in complex with its immunity protein, RhsI2  
Authors : Bullen, N.P.; Prehna, G.; Whitney, J.C.  
Deposited on : 2021-08-12  
Resolution : 2.49 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

<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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

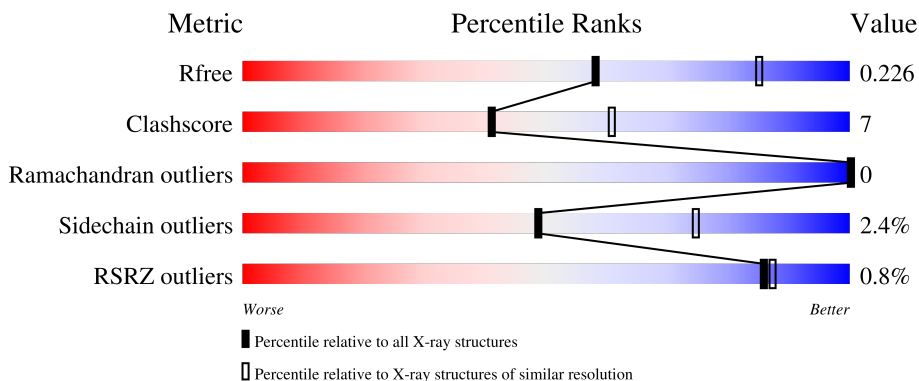
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	155	80% 12% 8%
1	B	155	79% 13% 8%
1	E	155	83% 9% 8%
1	G	155	68% 23% 8%
1	I	155	68% 21% 10%

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Mol	Chain	Length	Quality of chain
1	K	155	 82% 10% 8%
2	C	144	 85% 15%
2	D	144	 83% 17%
2	F	144	 3% 80% 19%
2	H	144	 1% 77% 21%
2	J	144	 86% 12%
2	L	144	 2% 80% 19%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27501 atoms, of which 13682 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 RhsP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	143	2198	698	1098	183	218	1	0	0	0
1	B	143	2198	698	1098	183	218	1	0	0	0
1	E	143	2198	698	1098	183	218	1	0	0	0
1	G	143	2198	698	1098	183	218	1	0	0	0
1	I	139	2159	687	1080	179	212	1	0	0	0
1	K	143	2198	698	1098	183	218	1	0	0	0

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1460	MET	-	expression tag	UNP A0A0H2Z8A2
A	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
A	1462	SER	-	expression tag	UNP A0A0H2Z8A2
A	1463	SER	-	expression tag	UNP A0A0H2Z8A2
A	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1466	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
A	1470	SER	-	expression tag	UNP A0A0H2Z8A2
A	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
A	1472	ASP	-	expression tag	UNP A0A0H2Z8A2
B	1460	MET	-	expression tag	UNP A0A0H2Z8A2
B	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
B	1462	SER	-	expression tag	UNP A0A0H2Z8A2
B	1463	SER	-	expression tag	UNP A0A0H2Z8A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1466	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
B	1470	SER	-	expression tag	UNP A0A0H2Z8A2
B	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
B	1472	ASP	-	expression tag	UNP A0A0H2Z8A2
E	1460	MET	-	expression tag	UNP A0A0H2Z8A2
E	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
E	1462	SER	-	expression tag	UNP A0A0H2Z8A2
E	1463	SER	-	expression tag	UNP A0A0H2Z8A2
E	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1466	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
E	1470	SER	-	expression tag	UNP A0A0H2Z8A2
E	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
E	1472	ASP	-	expression tag	UNP A0A0H2Z8A2
G	1460	MET	-	expression tag	UNP A0A0H2Z8A2
G	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
G	1462	SER	-	expression tag	UNP A0A0H2Z8A2
G	1463	SER	-	expression tag	UNP A0A0H2Z8A2
G	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1466	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
G	1470	SER	-	expression tag	UNP A0A0H2Z8A2
G	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
G	1472	ASP	-	expression tag	UNP A0A0H2Z8A2
I	1460	MET	-	expression tag	UNP A0A0H2Z8A2
I	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
I	1462	SER	-	expression tag	UNP A0A0H2Z8A2
I	1463	SER	-	expression tag	UNP A0A0H2Z8A2
I	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
I	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
I	1466	HIS	-	expression tag	UNP A0A0H2Z8A2

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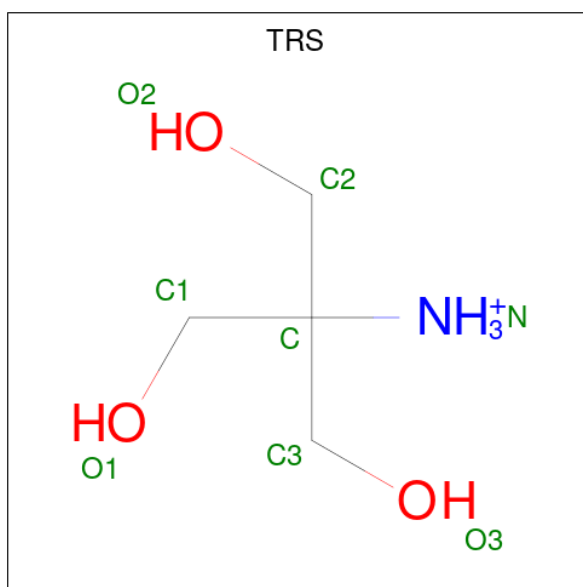
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Chain	Residue	Modelled	Actual	Comment	Reference
I	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
I	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
I	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
I	1470	SER	-	expression tag	UNP A0A0H2Z8A2
I	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
I	1472	ASP	-	expression tag	UNP A0A0H2Z8A2
K	1460	MET	-	expression tag	UNP A0A0H2Z8A2
K	1461	GLY	-	expression tag	UNP A0A0H2Z8A2
K	1462	SER	-	expression tag	UNP A0A0H2Z8A2
K	1463	SER	-	expression tag	UNP A0A0H2Z8A2
K	1464	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1465	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1466	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1467	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1468	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1469	HIS	-	expression tag	UNP A0A0H2Z8A2
K	1470	SER	-	expression tag	UNP A0A0H2Z8A2
K	1471	GLN	-	expression tag	UNP A0A0H2Z8A2
K	1472	ASP	-	expression tag	UNP A0A0H2Z8A2

- Molecule 2 is a protein called RhsI2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	144	Total	C	H	N	O	S	0	0	0
			2345	741	1179	193	230	2			
2	C	144	Total	C	H	N	O	S	0	0	0
			2345	741	1179	193	230	2			
2	F	144	Total	C	H	N	O	S	0	0	0
			2345	741	1179	193	230	2			
2	H	144	Total	C	H	N	O	S	0	0	0
			2346	741	1180	193	230	2			
2	J	144	Total	C	H	N	O	S	0	0	0
			2346	741	1180	193	230	2			
2	L	144	Total	C	H	N	O	S	0	0	0
			2345	741	1179	193	230	2			

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	A	1	20	4	12	1	3	0	0
3	D	1	20	4	12	1	3	0	0
3	C	1	20	4	12	1	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	D	17	Total	O	0	0
			17	17		
4	B	23	Total	O	0	0
			23	23		
4	C	17	Total	O	0	0
			17	17		
4	E	21	Total	O	0	0
			21	21		
4	F	23	Total	O	0	0
			23	23		
4	G	13	Total	O	0	0
			13	13		
4	H	17	Total	O	0	0
			17	17		
4	I	16	Total	O	0	0
			16	16		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	J	17	Total O 17 17	0	0
4	K	13	Total O 13 13	0	0
4	L	23	Total O 23 23	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: RhsP2

Chain A: 




- Molecule 1: RhsP2

Chain B: 



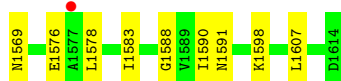
- Molecule 1: RhsP2

Chain E: 



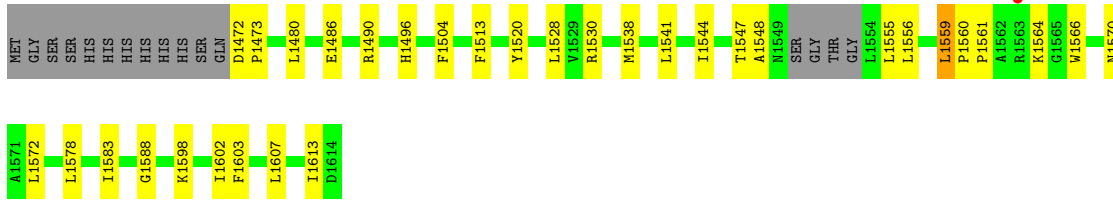
- Molecule 1: RhsP2

Chain G: 



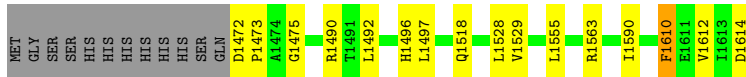
- Molecule 1: RhsP2

Chain I: 



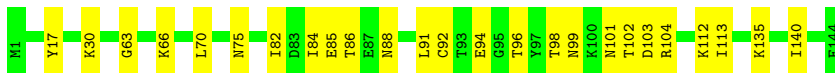
- Molecule 1: RhsP2

Chain K: 82% 10% 8%



- Molecule 2: RhsI2

Chain D: 83% 17%



- Molecule 2: RhsI2

Chain C: 85% 15%



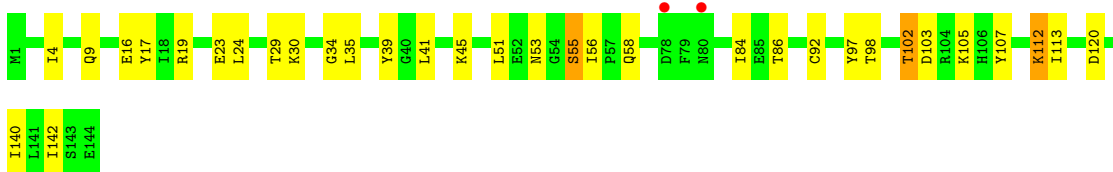
- Molecule 2: RhsI2

Chain F: 3% 80% 19%



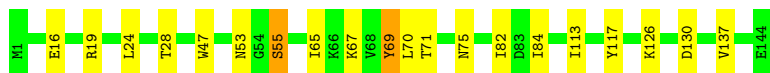
- Molecule 2: RhsI2

Chain H: 77% 21%

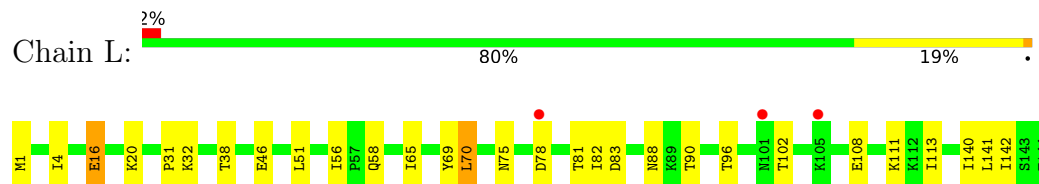


- Molecule 2: RhsI2

Chain J: 86% 12%



- Molecule 2: RhsI2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.46Å 112.46Å 324.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.39 – 2.49 97.39 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (97.39-2.49) 99.8 (97.39-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.195 , 0.232 0.193 , 0.226	Depositor DCC
$R_{free}$ test set	4261 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 12.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.440 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.333 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: TRS

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	0.27	0/1121	0.55	0/1522
1	B	0.26	0/1121	0.48	0/1522
1	E	0.26	0/1121	0.49	0/1522
1	G	0.27	0/1121	0.53	1/1522 (0.1%)
1	I	0.26	0/1099	0.49	0/1491
1	K	0.29	0/1121	0.52	0/1522
2	C	0.26	0/1188	0.48	0/1601
2	D	0.29	0/1188	0.50	0/1601
2	F	0.27	0/1188	0.50	0/1601
2	H	0.25	0/1188	0.47	0/1601
2	J	0.25	0/1188	0.48	0/1601
2	L	0.27	0/1188	0.50	0/1601
All	All	0.27	0/13832	0.50	1/18707 (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
1	K	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1563	ARG	CG-CD-NE	-5.48	100.29	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1563	ARG	Sidechain
1	K	1563	ARG	Sidechain

## 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	1100	1098	1098	12	0
1	B	1100	1098	1098	14	0
1	E	1100	1098	1098	10	0
1	G	1100	1098	1098	28	0
1	I	1079	1080	1079	23	0
1	K	1100	1098	1098	14	0
2	C	1166	1179	1179	15	0
2	D	1166	1179	1179	17	0
2	F	1166	1179	1179	20	0
2	H	1166	1180	1179	24	0
2	J	1166	1180	1179	12	0
2	L	1166	1179	1179	17	0
3	A	8	12	12	2	0
3	C	8	12	12	0	0
3	D	8	12	12	0	0
4	A	20	0	0	1	0
4	B	23	0	0	0	0
4	C	17	0	0	0	0
4	D	17	0	0	0	0
4	E	21	0	0	1	0
4	F	23	0	0	1	1
4	G	13	0	0	0	0
4	H	17	0	0	1	0
4	I	16	0	0	1	0
4	J	17	0	0	0	0
4	K	13	0	0	0	0
4	L	23	0	0	0	0
All	All	13819	13682	13679	193	1

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 7.

All (193) 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:I:1541:LEU:HD23	1:I:1602:ILE:HD11	1.58	0.86
2:C:71:THR:O	2:C:80:ASN:ND2	2.13	0.81
2:D:86:THR:OG1	2:D:88:ASN:OD1	1.99	0.81
2:C:80:ASN:OD1	2:C:81:THR:OG1	1.99	0.79
2:H:16:GLU:OE1	2:H:19:ARG:NH2	2.19	0.75
2:L:51:LEU:O	2:L:58:GLN:NE2	2.20	0.74
1:I:1548:ALA:HB2	1:I:1572:LEU:HD11	1.70	0.72
2:F:112:LYS:O	2:F:142:ILE:HD12	1.90	0.71
2:H:39:TYR:CG	2:H:56:ILE:HG22	2.25	0.70
2:C:35:LEU:HD22	2:C:120:ASP:HB3	1.74	0.68
1:G:1576:GLU:OE1	1:G:1591:ASN:ND2	2.27	0.68
2:C:79:PHE:CE2	2:C:104:ARG:HD2	2.29	0.67
1:B:1556:LEU:HB3	1:B:1559:LEU:HD13	1.77	0.66
1:G:1561:PRO:HG2	1:G:1563:ARG:HH22	1.59	0.66
1:B:1504:PHE:HB2	2:C:24:LEU:HD21	1.78	0.66
1:E:1529:VAL:HG22	1:E:1612:VAL:HG22	1.78	0.65
1:A:1517:LEU:HD22	3:A:1701:TRS:H21	1.80	0.64
2:C:82:ILE:HG23	2:C:96:THR:HG22	1.78	0.64
1:K:1610:PHE:CZ	1:K:1612:VAL:HG23	2.33	0.63
1:E:1504:PHE:HB2	2:F:24:LEU:HD21	1.81	0.63
1:B:1558:ASP:OD2	1:B:1559:LEU:HD12	1.99	0.62
2:H:53:ASN:OD1	2:H:55:SER:OG	2.15	0.62
1:B:1505:GLU:OE2	2:C:20:LYS:NZ	2.29	0.62
2:C:66:LYS:HE3	2:C:85:GLU:OE1	2.00	0.62
2:J:71:THR:O	2:J:75:ASN:ND2	2.33	0.62
2:L:113:ILE:HD11	2:L:140:ILE:HG23	1.80	0.62
2:D:98:THR:HG21	2:D:104:ARG:HA	1.82	0.61
1:K:1529:VAL:HG13	1:K:1610:PHE:CD1	2.35	0.61
2:L:1:MET:HB3	2:L:141:LEU:HD22	1.83	0.61
2:C:80:ASN:OD1	2:C:80:ASN:C	2.39	0.60
2:D:94:GLU:OE1	2:D:135:LYS:NZ	2.22	0.60
2:H:51:LEU:HD12	2:H:56:ILE:HD11	1.83	0.59
2:H:97:TYR:O	2:H:107:TYR:OH	2.20	0.57
1:I:1490:ARG:NH1	1:I:1513:PHE:O	2.37	0.57
1:I:1547:THR:HG22	1:I:1561:PRO:HA	1.85	0.57
2:H:45:LYS:HD3	2:L:46:GLU:HG3	1.87	0.57
1:I:1473:PRO:HG2	1:I:1555:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:THR:HG21	2:F:104:ARG:HA	1.87	0.56
1:K:1529:VAL:HG13	1:K:1610:PHE:HD1	1.70	0.56
2:H:51:LEU:CD1	2:H:56:ILE:HD11	2.35	0.56
1:I:1528:LEU:HD23	1:I:1613:ILE:HB	1.86	0.56
2:L:16:GLU:HG3	2:L:20:LYS:HD3	1.87	0.56
2:L:4:ILE:HA	2:L:102:THR:HG21	1.88	0.56
2:C:82:ILE:HG23	2:C:96:THR:CG2	2.35	0.56
2:H:35:LEU:HD22	2:H:120:ASP:HB3	1.86	0.55
2:C:8:LYS:HA	2:C:11:ILE:HD12	1.89	0.55
1:I:1530:ARG:NH1	1:I:1613:ILE:HD11	2.21	0.54
2:H:113:ILE:HD11	2:H:140:ILE:HG23	1.90	0.54
1:G:1481:ASP:N	1:G:1485:ASN:O	2.38	0.54
2:D:99:ASN:HB2	2:D:102:THR:HG23	1.88	0.54
1:B:1509:THR:O	1:B:1509:THR:HG23	2.07	0.53
2:H:84:ILE:N	2:H:92:CYS:O	2.41	0.53
1:K:1475:GLY:HA2	1:K:1590:ILE:HD12	1.91	0.53
1:A:1494:GLU:OE1	2:D:135:LYS:NZ	2.39	0.53
2:F:104:ARG:HB3	2:F:104:ARG:NH1	2.24	0.52
1:G:1547:THR:HB	1:G:1552:THR:HG23	1.91	0.52
2:H:24:LEU:HD23	2:H:24:LEU:O	2.09	0.52
1:K:1529:VAL:HG22	1:K:1610:PHE:HE1	1.74	0.52
1:A:1584:ASN:H	3:A:1701:TRS:H11	1.74	0.52
2:D:66:LYS:HG3	2:D:85:GLU:HB2	1.92	0.52
2:H:30:LYS:NZ	4:H:202:HOH:O	2.42	0.51
2:L:88:ASN:HB2	2:L:90:THR:HG22	1.91	0.51
2:F:70:LEU:HD21	2:F:75:ASN:OD1	2.11	0.51
1:E:1509:THR:O	1:E:1509:THR:HG23	2.11	0.51
2:H:24:LEU:HD22	2:H:34:GLY:HA3	1.92	0.50
2:J:16:GLU:OE2	2:J:19:ARG:NH2	2.39	0.50
1:I:1472:ASP:N	4:I:1702:HOH:O	2.45	0.50
1:K:1555:LEU:HD23	1:K:1555:LEU:O	2.12	0.50
1:B:1579:LYS:NZ	1:G:1557:PRO:O	2.34	0.50
2:J:53:ASN:OD1	2:J:55:SER:OG	2.26	0.50
2:D:113:ILE:HD11	2:D:140:ILE:HG23	1.94	0.49
1:E:1582:THR:HG23	1:G:1523:GLU:HA	1.93	0.49
2:F:71:THR:OG1	2:F:81:THR:HG21	2.11	0.49
1:G:1558:ASP:O	1:G:1559:LEU:HD23	2.12	0.49
1:K:1497:LEU:HD11	1:K:1610:PHE:HZ	1.77	0.49
1:I:1578:LEU:HD23	1:I:1588:GLY:HA3	1.95	0.49
1:B:1481:ASP:N	1:B:1485:ASN:O	2.39	0.49
2:L:113:ILE:HD12	2:L:141:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:GLU:HG3	2:C:20:LYS:HD2	1.94	0.49
2:J:117:TYR:HE1	2:J:137:VAL:HG22	1.77	0.49
2:F:98:THR:OG1	2:F:104:ARG:HG2	2.13	0.49
1:G:1503:ASN:HD21	2:H:17:TYR:HA	1.78	0.49
2:J:67:LYS:HD2	2:J:69:TYR:CD1	2.48	0.49
1:I:1504:PHE:HB2	2:J:24:LEU:HD21	1.94	0.48
2:L:31:PRO:O	2:L:32:LYS:HD3	2.13	0.48
1:G:1504:PHE:HB2	2:H:24:LEU:HD11	1.95	0.48
2:D:82:ILE:HG23	2:D:96:THR:HG22	1.94	0.48
2:H:4:ILE:O	2:H:102:THR:HG21	2.13	0.48
1:G:1509:THR:HG23	1:G:1509:THR:O	2.14	0.48
2:F:4:ILE:O	2:F:102:THR:HG21	2.14	0.48
1:A:1509:THR:O	1:A:1509:THR:HG23	2.14	0.48
2:L:56:ILE:O	2:L:58:GLN:HG3	2.14	0.48
1:A:1545:GLY:O	1:A:1559:LEU:HD22	2.14	0.48
2:F:57:PRO:HG2	2:F:119:PHE:HB2	1.96	0.47
2:H:39:TYR:CD2	2:H:56:ILE:HG22	2.48	0.47
2:L:65:ILE:HD11	2:L:142:ILE:HD11	1.96	0.47
1:I:1530:ARG:HH12	1:I:1613:ILE:HD11	1.79	0.47
2:F:19:ARG:NH1	2:F:23:GLU:OE2	2.48	0.47
1:I:1564:LYS:HD3	1:I:1564:LYS:C	2.35	0.47
2:F:68:VAL:HG22	2:F:82:ILE:HG22	1.97	0.47
1:A:1575:LEU:HD21	1:A:1578:LEU:HD11	1.97	0.47
1:E:1481:ASP:HB3	1:E:1483:GLN:H	1.80	0.47
2:F:1:MET:HE1	2:F:112:LYS:O	2.14	0.47
1:E:1493:SER:CB	2:F:80:ASN:OD1	2.63	0.47
2:D:63:GLY:O	2:D:112:LYS:HG2	2.16	0.46
1:I:1544:ILE:HD13	1:I:1598:LYS:HD3	1.98	0.46
1:I:1538:MET:HA	1:I:1541:LEU:HD12	1.98	0.46
2:L:69:TYR:OH	2:L:83:ASP:OD1	2.25	0.46
2:F:70:LEU:HD23	2:F:71:THR:N	2.31	0.46
1:G:1578:LEU:HD23	1:G:1588:GLY:HA3	1.97	0.46
1:A:1490:ARG:HG2	1:A:1492:LEU:CD1	2.46	0.45
2:F:94:GLU:OE1	2:F:135:LYS:NZ	2.36	0.45
2:J:117:TYR:CE1	2:J:137:VAL:HG22	2.51	0.45
1:K:1555:LEU:HD13	1:K:1590:ILE:HD11	1.97	0.45
1:I:1566:TRP:HB2	1:I:1570:ASN:HB2	1.97	0.45
1:G:1556:LEU:HB3	1:G:1559:LEU:HD12	1.98	0.45
1:G:1569:ASN:OD1	1:G:1598:LYS:HE3	2.17	0.45
1:A:1490:ARG:HG2	1:A:1492:LEU:HD12	1.99	0.45
1:B:1572:LEU:O	1:B:1593:GLY:N	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1555:LEU:HD13	1:G:1590:ILE:HD11	1.99	0.45
1:G:1561:PRO:CG	1:G:1563:ARG:HH22	2.27	0.45
1:I:1472:ASP:N	1:I:1473:PRO:HD2	2.31	0.45
1:G:1539:ASN:O	1:G:1543:LYS:HG2	2.17	0.45
1:K:1518:GLN:HG3	1:K:1528:LEU:HD21	1.99	0.44
1:I:1556:LEU:HB2	1:I:1559:LEU:HD12	1.98	0.44
1:K:1472:ASP:N	1:K:1473:PRO:CD	2.80	0.44
2:D:101:ASN:O	2:D:101:ASN:OD1	2.35	0.44
2:H:98:THR:HB	2:H:102:THR:HG22	1.99	0.44
2:D:84:ILE:HD13	2:D:113:ILE:HG12	1.99	0.44
2:J:65:ILE:HD11	2:J:113:ILE:HD13	2.00	0.43
1:G:1517:LEU:CD2	1:G:1583:ILE:HD12	2.48	0.43
1:A:1472:ASP:N	4:A:1806:HOH:O	2.51	0.43
1:A:1502:ASN:ND2	2:D:17:TYR:OH	2.42	0.43
1:I:1520:TYR:HA	1:I:1583:ILE:HD13	1.99	0.43
2:J:70:LEU:HD11	2:J:75:ASN:HB3	1.99	0.43
2:H:56:ILE:O	2:H:58:GLN:HG3	2.19	0.43
1:G:1532:THR:O	1:G:1607:LEU:HD12	2.19	0.43
2:D:91:LEU:HD22	2:D:92:CYS:N	2.34	0.43
2:F:99:ASN:H	2:F:102:THR:CG2	2.32	0.43
1:G:1556:LEU:CB	1:G:1559:LEU:HD12	2.49	0.43
2:J:82:ILE:HD12	2:J:84:ILE:HD11	2.00	0.43
2:D:70:LEU:HD21	2:D:75:ASN:HB2	2.00	0.43
1:E:1472:ASP:O	1:E:1584:ASN:ND2	2.48	0.43
1:G:1556:LEU:HD13	1:G:1559:LEU:CD1	2.49	0.42
1:I:1578:LEU:HD23	1:I:1588:GLY:CA	2.49	0.42
1:K:1497:LEU:HD11	1:K:1610:PHE:CZ	2.54	0.42
1:B:1500:LEU:O	1:B:1504:PHE:HA	2.20	0.42
2:C:27:ASN:OD1	2:C:30:LYS:HB2	2.19	0.42
2:C:51:LEU:HA	2:C:56:ILE:HG22	2.00	0.42
2:L:70:LEU:HD21	2:L:75:ASN:HB2	2.01	0.42
2:H:113:ILE:HD11	2:H:140:ILE:CG2	2.48	0.42
1:I:1559:LEU:HD23	1:I:1560:PRO:HD2	2.01	0.42
1:B:1580:LYS:HD2	1:B:1580:LYS:HA	1.92	0.42
2:F:37:GLY:N	4:F:203:HOH:O	2.47	0.42
1:G:1517:LEU:HD22	1:G:1583:ILE:CD1	2.50	0.42
2:F:41:LEU:O	2:F:47:TRP:HB2	2.20	0.42
2:F:104:ARG:CZ	2:F:104:ARG:CB	2.98	0.42
2:J:28:THR:O	2:J:28:THR:HG22	2.19	0.42
1:E:1558:ASP:OD1	4:E:1701:HOH:O	2.22	0.42
1:G:1516:PRO:C	1:G:1517:LEU:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:MET:HB3	2:L:141:LEU:HB3	2.02	0.42
1:G:1478:VAL:HG22	1:G:1516:PRO:HB2	2.01	0.42
1:K:1490:ARG:HG2	1:K:1492:LEU:HD23	2.02	0.42
2:D:30:LYS:HA	2:D:30:LYS:HD2	1.78	0.41
1:A:1472:ASP:N	1:A:1473:PRO:CD	2.83	0.41
1:I:1603:PHE:O	1:I:1607:LEU:N	2.53	0.41
1:B:1472:ASP:N	1:B:1473:PRO:CD	2.83	0.41
2:F:98:THR:HG21	2:F:104:ARG:HG2	2.03	0.41
2:D:82:ILE:HG23	2:D:96:THR:CG2	2.50	0.41
1:G:1578:LEU:HD23	1:G:1588:GLY:CA	2.50	0.41
1:G:1472:ASP:N	1:G:1473:PRO:CD	2.83	0.41
2:H:41:LEU:HD11	2:L:38:THR:CG2	2.51	0.41
1:B:1527:LYS:HD2	1:B:1527:LYS:HA	1.92	0.41
1:B:1529:VAL:HA	1:B:1611:GLU:O	2.21	0.41
1:G:1480:LEU:HD23	1:G:1486:GLU:HA	2.02	0.41
2:H:112:LYS:CA	2:H:112:LYS:HE2	2.49	0.41
2:J:126:LYS:HD2	2:J:130:ASP:HB2	2.02	0.41
1:E:1598:LYS:O	1:E:1602:ILE:HG12	2.20	0.41
2:H:112:LYS:HE2	2:H:112:LYS:HA	2.02	0.41
1:K:1529:VAL:HG13	1:K:1610:PHE:CE1	2.56	0.41
1:A:1577:ALA:HB1	1:A:1583:ILE:HD12	2.02	0.40
2:D:101:ASN:OD1	2:D:101:ASN:C	2.60	0.40
1:E:1545:GLY:O	1:E:1559:LEU:HD22	2.22	0.40
1:G:1497:LEU:HD22	1:G:1527:LYS:HG3	2.03	0.40
1:G:1548:ALA:H	1:G:1552:THR:HG21	1.86	0.40
2:L:82:ILE:HG23	2:L:96:THR:CG2	2.51	0.40
1:K:1610:PHE:HZ	1:K:1612:VAL:HG23	1.85	0.40
2:L:108:GLU:HB2	2:L:111:LYS:HE3	2.02	0.40
1:B:1492:LEU:HD12	1:B:1492:LEU:N	2.36	0.40
2:C:70:LEU:HD21	2:C:75:ASN:HB2	2.03	0.40
2:H:29:THR:O	2:H:29:THR:CG2	2.69	0.40
1:I:1480:LEU:HD23	1:I:1486:GLU:HA	2.04	0.40
1:I:1556:LEU:O	1:I:1559:LEU:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:222:HOH:O	4:F:223:HOH:O[4_645]	2.02	0.18

## 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	141/155 (91%)	134 (95%)	7 (5%)	0	100	100
1	B	141/155 (91%)	132 (94%)	9 (6%)	0	100	100
1	E	141/155 (91%)	131 (93%)	10 (7%)	0	100	100
1	G	141/155 (91%)	133 (94%)	8 (6%)	0	100	100
1	I	135/155 (87%)	129 (96%)	6 (4%)	0	100	100
1	K	141/155 (91%)	131 (93%)	10 (7%)	0	100	100
2	C	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
2	D	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
2	F	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
2	H	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
2	J	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
2	L	142/144 (99%)	142 (100%)	0	0	100	100
All	All	1692/1794 (94%)	1635 (97%)	57 (3%)	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	121/132 (92%)	118 (98%)	3 (2%)	47	73
1	B	121/132 (92%)	120 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	121/132 (92%)	120 (99%)	1 (1%)	81	93
1	G	121/132 (92%)	118 (98%)	3 (2%)	47	73
1	I	119/132 (90%)	117 (98%)	2 (2%)	60	82
1	K	121/132 (92%)	118 (98%)	3 (2%)	47	73
2	C	130/130 (100%)	129 (99%)	1 (1%)	81	93
2	D	130/130 (100%)	129 (99%)	1 (1%)	81	93
2	F	130/130 (100%)	125 (96%)	5 (4%)	33	58
2	H	130/130 (100%)	121 (93%)	9 (7%)	15	30
2	J	130/130 (100%)	127 (98%)	3 (2%)	50	76
2	L	130/130 (100%)	126 (97%)	4 (3%)	40	67
All	All	1504/1572 (96%)	1468 (98%)	36 (2%)	49	74

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

Mol	Chain	Res	Type
1	A	1558	ASP
1	A	1569	ASN
1	A	1582	THR
2	D	103	ASP
1	B	1563	ARG
2	C	80	ASN
1	E	1481	ASP
2	F	29	THR
2	F	58	GLN
2	F	69	TYR
2	F	81	THR
2	F	126	LYS
1	G	1481	ASP
1	G	1519	SER
1	G	1563	ARG
2	H	9	GLN
2	H	23	GLU
2	H	55	SER
2	H	86	THR
2	H	102	THR
2	H	103	ASP
2	H	105	LYS
2	H	112	LYS

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Mol	Chain	Res	Type
2	H	142	ILE
1	I	1496	HIS
1	I	1559	LEU
2	J	47	TRP
2	J	55	SER
2	J	69	TYR
1	K	1496	HIS
1	K	1610	PHE
1	K	1614	ASP
2	L	16	GLU
2	L	70	LEU
2	L	78	ASP
2	L	81	THR

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

Mol	Chain	Res	Type
2	C	58	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TRS	A	1701	-	7,7,7	0.42	0	9,9,9	1.42	2 (22%)
3	TRS	C	201	-	7,7,7	0.37	0	9,9,9	1.19	1 (11%)
3	TRS	D	201	-	7,7,7	0.33	0	9,9,9	1.09	2 (22%)

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
3	TRS	A	1701	-	-	3/9/9/9	-
3	TRS	C	201	-	-	1/9/9/9	-
3	TRS	D	201	-	-	0/9/9/9	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1701	TRS	C2-C-C1	-2.72	102.38	110.81
3	A	1701	TRS	C2-C-N	2.50	115.43	107.98
3	C	201	TRS	C1-C-N	2.34	114.95	107.98
3	D	201	TRS	C2-C-C1	-2.06	104.41	110.81
3	D	201	TRS	C2-C-N	2.02	114.01	107.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	TRS	N-C-C2-O2
3	A	1701	TRS	C1-C-C2-O2
3	A	1701	TRS	N-C-C2-O2
3	A	1701	TRS	C3-C-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1701	TRS	2	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, 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	143/155 (92%)	-0.30	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	34, 43, 58, 79	0
1	B	143/155 (92%)	-0.22	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	35, 44, 59, 87	0
1	E	143/155 (92%)	-0.14	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">89</span>	34, 48, 62, 72	0
1	G	143/155 (92%)	-0.10	2 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">77</span>	37, 49, 69, 82	0
1	I	139/155 (89%)	-0.09	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">89</span>	34, 47, 66, 81	0
1	K	143/155 (92%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	34, 45, 66, 79	0
2	C	144/144 (100%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	29, 43, 64, 76	0
2	D	144/144 (100%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	33, 45, 65, 83	0
2	F	144/144 (100%)	-0.11	4 (2%) <span style="border: 1px solid blue; padding: 2px;">53</span> <span style="border: 1px solid blue; padding: 2px;">56</span>	33, 47, 65, 81	0
2	H	144/144 (100%)	-0.17	2 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">77</span>	34, 49, 68, 78	0
2	J	144/144 (100%)	-0.25	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	29, 42, 58, 74	0
2	L	144/144 (100%)	-0.20	3 (2%) <span style="border: 1px solid blue; padding: 2px;">63</span> <span style="border: 1px solid blue; padding: 2px;">66</span>	30, 43, 71, 76	0
All	All	1718/1794 (95%)	-0.19	13 (0%) <span style="border: 1px solid blue; padding: 2px;">86</span> <span style="border: 1px solid blue; padding: 2px;">87</span>	29, 46, 66, 87	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1614	ASP	3.7
2	L	78	ASP	3.1
1	I	1563	ARG	3.1
2	F	100	LYS	2.7
2	F	76	THR	2.7
2	F	103	ASP	2.7
2	H	80	ASN	2.5
2	H	78	ASP	2.4
1	G	1472	ASP	2.4
2	F	101	ASN	2.1
1	G	1577	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	101	ASN	2.0
2	L	105	LYS	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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	TRS	C	201	8/8	0.77	0.24	30,41,51,51	0
3	TRS	A	1701	8/8	0.89	0.17	24,36,48,48	0
3	TRS	D	201	8/8	0.92	0.11	29,39,44,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.