



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 01:44 PM EST

PDB ID : 2OGE  
Title : x-ray structure of *S. venezuelae* DesV in its internal aldimine form  
Authors : Holden, H.M.; Burgie, E.S.  
Deposited on : 2007-01-05  
Resolution : 2.05 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>.

---

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 : 2.36  
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) : 2.36

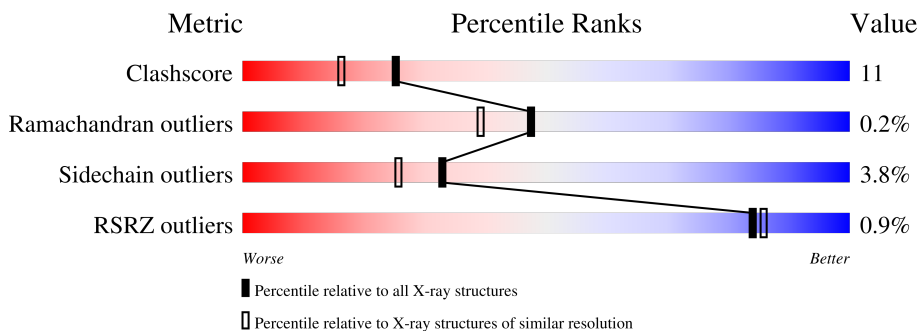
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	399	 % 60% 27% 5% 8%
1	B	399	 % 65% 22% 5% 8%
1	C	399	 % 66% 23% 8%
1	D	399	 % 60% 28% 8%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12743 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 Transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	368	2840	1783	520	530	1	6	0	0	0
1	B	369	2847	1788	521	531	1	6	0	0	0
1	C	369	2847	1788	521	531	1	6	0	0	0
1	D	368	2840	1783	520	530	1	6	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9ZGH4
A	-18	GLY	-	cloning artifact	UNP Q9ZGH4
A	-17	SER	-	cloning artifact	UNP Q9ZGH4
A	-16	SER	-	cloning artifact	UNP Q9ZGH4
A	-15	HIS	-	expression tag	UNP Q9ZGH4
A	-14	HIS	-	expression tag	UNP Q9ZGH4
A	-13	HIS	-	expression tag	UNP Q9ZGH4
A	-12	HIS	-	expression tag	UNP Q9ZGH4
A	-11	HIS	-	expression tag	UNP Q9ZGH4
A	-10	HIS	-	expression tag	UNP Q9ZGH4
A	-9	SER	-	cloning artifact	UNP Q9ZGH4
A	-8	SER	-	cloning artifact	UNP Q9ZGH4
A	-7	GLU	-	cloning artifact	UNP Q9ZGH4
A	-6	ASN	-	cloning artifact	UNP Q9ZGH4
A	-5	LEU	-	cloning artifact	UNP Q9ZGH4
A	-4	TYR	-	cloning artifact	UNP Q9ZGH4
A	-3	PHE	-	cloning artifact	UNP Q9ZGH4
A	-2	GLN	-	cloning artifact	UNP Q9ZGH4
A	-1	GLY	-	cloning artifact	UNP Q9ZGH4
A	0	HIS	-	cloning artifact	UNP Q9ZGH4
B	-19	MET	-	initiating methionine	UNP Q9ZGH4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	cloning artifact	UNP Q9ZGH4
B	-17	SER	-	cloning artifact	UNP Q9ZGH4
B	-16	SER	-	cloning artifact	UNP Q9ZGH4
B	-15	HIS	-	expression tag	UNP Q9ZGH4
B	-14	HIS	-	expression tag	UNP Q9ZGH4
B	-13	HIS	-	expression tag	UNP Q9ZGH4
B	-12	HIS	-	expression tag	UNP Q9ZGH4
B	-11	HIS	-	expression tag	UNP Q9ZGH4
B	-10	HIS	-	expression tag	UNP Q9ZGH4
B	-9	SER	-	cloning artifact	UNP Q9ZGH4
B	-8	SER	-	cloning artifact	UNP Q9ZGH4
B	-7	GLU	-	cloning artifact	UNP Q9ZGH4
B	-6	ASN	-	cloning artifact	UNP Q9ZGH4
B	-5	LEU	-	cloning artifact	UNP Q9ZGH4
B	-4	TYR	-	cloning artifact	UNP Q9ZGH4
B	-3	PHE	-	cloning artifact	UNP Q9ZGH4
B	-2	GLN	-	cloning artifact	UNP Q9ZGH4
B	-1	GLY	-	cloning artifact	UNP Q9ZGH4
B	0	HIS	-	cloning artifact	UNP Q9ZGH4
C	-19	MET	-	initiating methionine	UNP Q9ZGH4
C	-18	GLY	-	cloning artifact	UNP Q9ZGH4
C	-17	SER	-	cloning artifact	UNP Q9ZGH4
C	-16	SER	-	cloning artifact	UNP Q9ZGH4
C	-15	HIS	-	expression tag	UNP Q9ZGH4
C	-14	HIS	-	expression tag	UNP Q9ZGH4
C	-13	HIS	-	expression tag	UNP Q9ZGH4
C	-12	HIS	-	expression tag	UNP Q9ZGH4
C	-11	HIS	-	expression tag	UNP Q9ZGH4
C	-10	HIS	-	expression tag	UNP Q9ZGH4
C	-9	SER	-	cloning artifact	UNP Q9ZGH4
C	-8	SER	-	cloning artifact	UNP Q9ZGH4
C	-7	GLU	-	cloning artifact	UNP Q9ZGH4
C	-6	ASN	-	cloning artifact	UNP Q9ZGH4
C	-5	LEU	-	cloning artifact	UNP Q9ZGH4
C	-4	TYR	-	cloning artifact	UNP Q9ZGH4
C	-3	PHE	-	cloning artifact	UNP Q9ZGH4
C	-2	GLN	-	cloning artifact	UNP Q9ZGH4
C	-1	GLY	-	cloning artifact	UNP Q9ZGH4
C	0	HIS	-	cloning artifact	UNP Q9ZGH4
D	-19	MET	-	initiating methionine	UNP Q9ZGH4
D	-18	GLY	-	cloning artifact	UNP Q9ZGH4
D	-17	SER	-	cloning artifact	UNP Q9ZGH4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	cloning artifact	UNP Q9ZGH4
D	-15	HIS	-	expression tag	UNP Q9ZGH4
D	-14	HIS	-	expression tag	UNP Q9ZGH4
D	-13	HIS	-	expression tag	UNP Q9ZGH4
D	-12	HIS	-	expression tag	UNP Q9ZGH4
D	-11	HIS	-	expression tag	UNP Q9ZGH4
D	-10	HIS	-	expression tag	UNP Q9ZGH4
D	-9	SER	-	cloning artifact	UNP Q9ZGH4
D	-8	SER	-	cloning artifact	UNP Q9ZGH4
D	-7	GLU	-	cloning artifact	UNP Q9ZGH4
D	-6	ASN	-	cloning artifact	UNP Q9ZGH4
D	-5	LEU	-	cloning artifact	UNP Q9ZGH4
D	-4	TYR	-	cloning artifact	UNP Q9ZGH4
D	-3	PHE	-	cloning artifact	UNP Q9ZGH4
D	-2	GLN	-	cloning artifact	UNP Q9ZGH4
D	-1	GLY	-	cloning artifact	UNP Q9ZGH4
D	0	HIS	-	cloning artifact	UNP Q9ZGH4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	2	Total Cl 2 2	0	0
2	C	2	Total Cl 2 2	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 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
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

*Continued on next page...*

*Continued from previous page...*

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

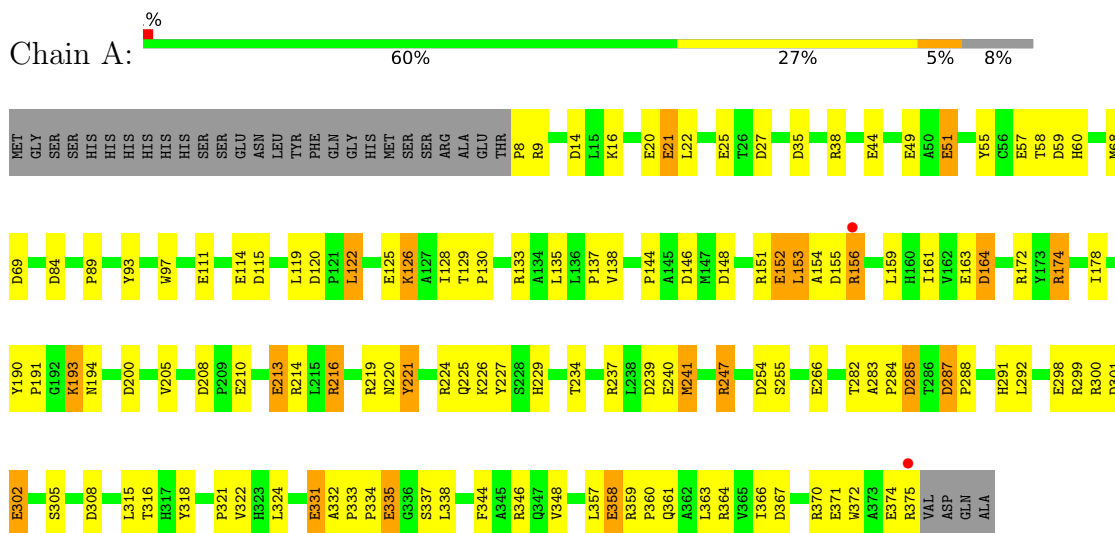
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	342	Total O 342 342	0	0
5	B	302	Total O 302 302	0	0
5	C	330	Total O 330 330	0	0
5	D	301	Total O 301 301	0	0

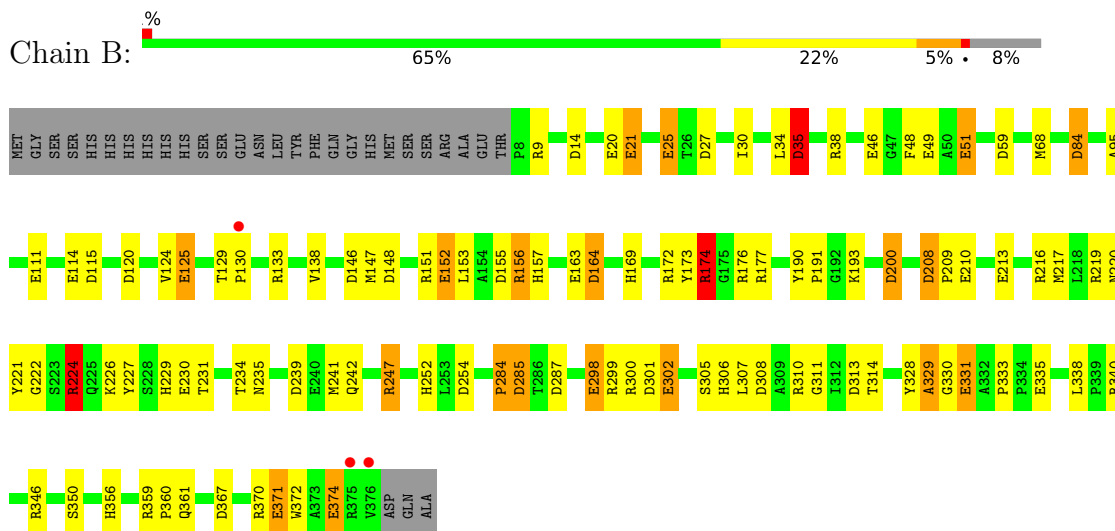
### 3 Residue-property plots

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: Transaminase



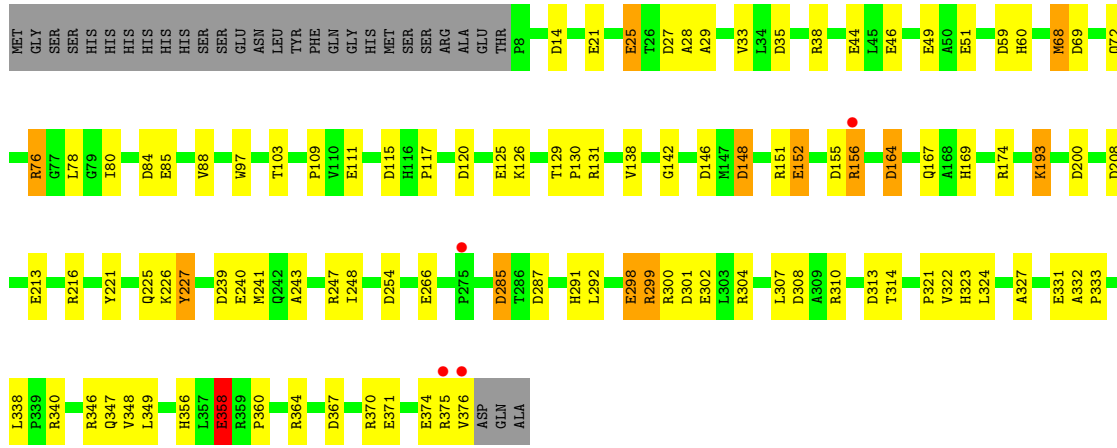
- Molecule 1: Transaminase



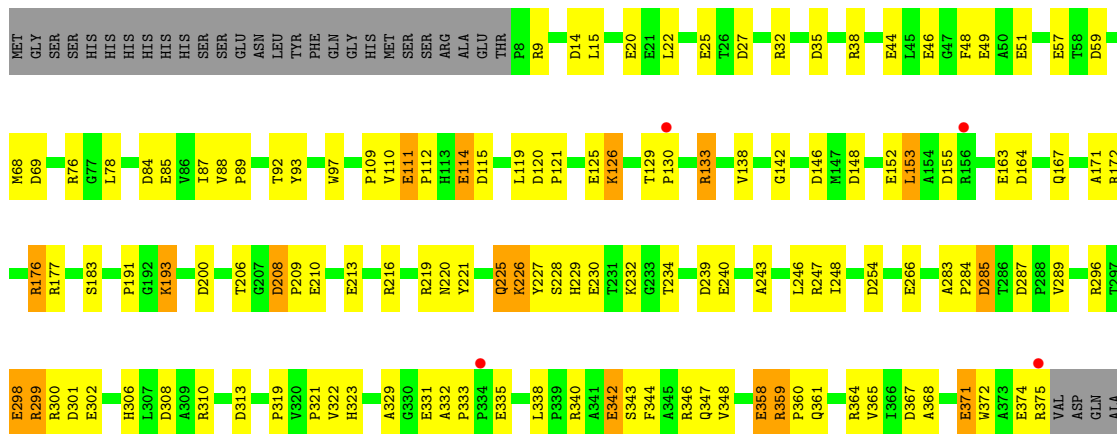
- Molecule 1: Transaminase







• Molecule 1: Transaminase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.80Å 143.82Å 81.13Å 90.00° 106.95° 90.00°	Depositor
Resolution (Å)	30.50 – 2.05 30.51 – 2.05	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.50-2.05) 94.0 (30.51-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.89 (at 2.05Å)	Xtrriage
Refinement program	REFMAC, TNT	Depositor
R, $R_{free}$	0.159 , 0.234 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtrriage
Anisotropy	0.469	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 91.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5835e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, LLP, EDO, NA

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	0.87	22/2886 (0.8%)	1.30	46/3932 (1.2%)
1	B	0.86	19/2893 (0.7%)	1.28	45/3942 (1.1%)
1	C	0.86	17/2893 (0.6%)	1.31	50/3942 (1.3%)
1	D	0.87	26/2886 (0.9%)	1.27	46/3932 (1.2%)
All	All	0.86	84/11558 (0.7%)	1.29	187/15748 (1.2%)

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	GLU	CD-OE2	6.53	1.32	1.25
1	D	25	GLU	CD-OE2	6.46	1.32	1.25
1	A	57	GLU	CD-OE2	6.28	1.32	1.25
1	D	374	GLU	CD-OE2	6.18	1.32	1.25
1	D	298	GLU	CD-OE2	6.10	1.32	1.25
1	A	213	GLU	CD-OE2	6.06	1.32	1.25
1	C	111	GLU	CD-OE2	6.04	1.32	1.25
1	C	374	GLU	CD-OE2	5.96	1.32	1.25
1	B	213	GLU	CD-OE2	5.92	1.32	1.25
1	B	111	GLU	CD-OE2	5.88	1.32	1.25
1	B	298	GLU	CD-OE2	5.87	1.32	1.25
1	C	371	GLU	CD-OE2	5.87	1.32	1.25
1	D	335	GLU	CD-OE2	5.87	1.32	1.25
1	B	331	GLU	CD-OE2	5.85	1.32	1.25
1	A	358	GLU	CD-OE2	5.84	1.32	1.25
1	A	240	GLU	CD-OE2	5.83	1.32	1.25
1	B	152	GLU	CD-OE2	5.83	1.32	1.25
1	A	25	GLU	CD-OE2	5.83	1.32	1.25
1	A	298	GLU	CD-OE2	5.82	1.32	1.25
1	C	51	GLU	CD-OE2	5.78	1.32	1.25
1	A	210	GLU	CD-OE2	5.75	1.31	1.25
1	D	240	GLU	CD-OE2	5.75	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CD-OE2	5.74	1.31	1.25
1	B	21	GLU	CD-OE2	5.73	1.31	1.25
1	D	371	GLU	CD-OE2	5.68	1.31	1.25
1	A	374	GLU	CD-OE2	5.68	1.31	1.25
1	A	125	GLU	CD-OE2	5.67	1.31	1.25
1	B	302	GLU	CD-OE2	5.67	1.31	1.25
1	D	111	GLU	CD-OE2	5.67	1.31	1.25
1	A	49	GLU	CD-OE2	5.66	1.31	1.25
1	D	213	GLU	CD-OE2	5.65	1.31	1.25
1	B	371	GLU	CD-OE2	5.64	1.31	1.25
1	D	342	GLU	CD-OE2	5.64	1.31	1.25
1	C	331	GLU	CD-OE2	5.64	1.31	1.25
1	A	51	GLU	CD-OE2	5.63	1.31	1.25
1	D	49	GLU	CD-OE2	5.62	1.31	1.25
1	B	374	GLU	CD-OE2	5.61	1.31	1.25
1	D	114	GLU	CD-OE2	5.60	1.31	1.25
1	D	210	GLU	CD-OE2	5.58	1.31	1.25
1	C	152	GLU	CD-OE2	5.57	1.31	1.25
1	C	125	GLU	CD-OE2	5.56	1.31	1.25
1	C	25	GLU	CD-OE2	5.53	1.31	1.25
1	C	240	GLU	CD-OE2	5.49	1.31	1.25
1	D	302	GLU	CD-OE2	5.49	1.31	1.25
1	D	230	GLU	CD-OE2	5.47	1.31	1.25
1	A	335	GLU	CD-OE2	5.47	1.31	1.25
1	B	46	GLU	CD-OE2	5.46	1.31	1.25
1	D	163	GLU	CD-OE2	5.46	1.31	1.25
1	D	125	GLU	CD-OE2	5.46	1.31	1.25
1	B	20	GLU	CD-OE2	5.43	1.31	1.25
1	D	266	GLU	CD-OE2	5.43	1.31	1.25
1	B	210	GLU	CD-OE2	5.42	1.31	1.25
1	C	358	GLU	CD-OE2	5.41	1.31	1.25
1	A	21	GLU	CD-OE2	5.38	1.31	1.25
1	C	213	GLU	CD-OE2	5.38	1.31	1.25
1	D	85	GLU	CD-OE2	5.38	1.31	1.25
1	A	20	GLU	CD-OE2	5.37	1.31	1.25
1	C	46	GLU	CD-OE2	5.35	1.31	1.25
1	A	302	GLU	CD-OE2	5.33	1.31	1.25
1	D	152	GLU	CD-OE2	5.30	1.31	1.25
1	C	85	GLU	CD-OE2	5.28	1.31	1.25
1	B	125	GLU	CD-OE2	5.26	1.31	1.25
1	D	358	GLU	CD-OE2	5.25	1.31	1.25
1	B	335	GLU	CD-OE2	5.24	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	GLU	CD-OE2	5.24	1.31	1.25
1	D	331	GLU	CD-OE2	5.24	1.31	1.25
1	D	44	GLU	CD-OE2	5.23	1.31	1.25
1	B	114	GLU	CD-OE2	5.21	1.31	1.25
1	D	46	GLU	CD-OE2	5.18	1.31	1.25
1	D	51	GLU	CD-OE2	5.17	1.31	1.25
1	C	298	GLU	CD-OE2	5.16	1.31	1.25
1	A	331	GLU	CD-OE2	5.15	1.31	1.25
1	B	25	GLU	CD-OE2	5.14	1.31	1.25
1	C	302	GLU	CD-OE2	5.14	1.31	1.25
1	A	152	GLU	CD-OE2	5.13	1.31	1.25
1	D	20	GLU	CD-OE2	5.11	1.31	1.25
1	B	49	GLU	CD-OE2	5.09	1.31	1.25
1	A	44	GLU	CD-OE2	5.07	1.31	1.25
1	A	163	GLU	CD-OE2	5.07	1.31	1.25
1	A	111	GLU	CD-OE2	5.06	1.31	1.25
1	D	57	GLU	CD-OE2	5.05	1.31	1.25
1	B	51	GLU	CD-OE2	5.04	1.31	1.25
1	A	266	GLU	CD-OE2	5.02	1.31	1.25
1	B	163	GLU	CD-OE2	5.00	1.31	1.25

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	ASP	CB-CG-OD1	10.13	127.42	118.30
1	B	224	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	B	239	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	C	340	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	C	76	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	247	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	C	120	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	A	247	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	C	239	ASP	CB-CG-OD2	-8.53	110.63	118.30
1	C	254	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	C	27	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	D	76	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	216	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	285	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	B	340	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	D	219	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	247	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	A	239	ASP	CB-CG-OD2	-7.94	111.16	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	174	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	D	27	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	14	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	308	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	208	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	B	285	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	27	ASP	CB-CG-OD1	7.46	125.02	118.30
1	D	239	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	D	120	ASP	CB-CG-OD1	7.44	124.99	118.30
1	C	146	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	35	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	D	208	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	247	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	14	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	120	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	D	146	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	C	208	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	301	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	367	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	C	239	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	285	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	C	35	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	208	ASP	CB-CG-OD1	7.05	124.64	118.30
1	C	200	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	254	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	14	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	285	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	120	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	200	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	27	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	C	254	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	200	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	146	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	27	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	301	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	177	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	224	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	301	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	200	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	D	200	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	D	287	ASP	CB-CG-OD2	-6.70	112.27	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	B	208	ASP	CB-CG-OD1	6.67	124.30	118.30
1	C	370	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	35	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	115	ASP	CB-CG-OD1	6.57	124.21	118.30
1	D	32	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	D	208	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	308	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	148	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	120	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	221	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	D	367	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	146	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	D	35	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	146	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	27	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	287	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	27	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	B	254	ASP	CB-CG-OD1	6.43	124.08	118.30
1	B	115	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	155	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	C	155	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	308	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	C	148	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	14	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	120	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	120	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	177	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	59	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	D	301	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	164	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	367	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	69	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	164	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	287	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	239	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	313	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	308	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	32	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	367	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	D	148	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	200	ASP	CB-CG-OD1	6.16	123.84	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	115	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	254	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	367	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	14	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	148	ASP	CB-CG-OD1	6.03	123.72	118.30
1	D	313	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	301	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	300	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	301	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	285	ASP	CB-CG-OD1	5.98	123.68	118.30
1	D	115	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	296	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	84	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	B	84	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	B	146	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	208	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	27	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	59	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	69	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	69	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	308	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	313	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	254	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	59	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	155	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	148	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	367	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	156	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	308	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	D	239	ASP	CB-CG-OD1	5.73	123.45	118.30
1	B	285	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	84	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	164	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	200	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	35	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	301	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	148	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	115	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	224	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	9	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	219	ARG	NE-CZ-NH1	5.63	123.11	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	287	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	313	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	254	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	155	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	164	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	200	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	14	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	35	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	174	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	298	GLU	N-CA-C	-5.51	96.12	111.00
1	D	364	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	146	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	14	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	300	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	164	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	D	69	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	120	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	148	ASP	CB-CG-OD1	5.38	123.15	118.30
1	B	155	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	148	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	59	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	219	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	287	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	346	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	304	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	340	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	177	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	364	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	151	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	35	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	216	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	340	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	155	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	300	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	285	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	115	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	69	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	146	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	364	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	227	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	214	ARG	NE-CZ-NH1	5.05	122.83	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2840	0	2780	80	0
1	B	2847	0	2789	69	0
1	C	2847	0	2789	60	0
1	D	2840	0	2780	64	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	33	4	0
4	B	12	0	16	1	0
4	C	20	0	21	3	0
4	D	24	0	26	5	0
5	A	342	0	0	5	0
5	B	302	0	0	7	0
5	C	330	0	0	8	0
5	D	301	0	0	3	0
All	All	12743	0	11234	243	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 11.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HB2	4:D:1310:EDO:H11	1.38	1.05

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:MET:HE3	1:D:234:THR:HA	1.54	0.89
1:C:299:ARG:HG2	1:C:299:ARG:HH11	1.39	0.87
1:B:306:HIS:CD2	1:B:372:TRP:HB2	2.21	0.77
1:A:315:LEU:HD22	1:B:226:LYS:HE2	1.68	0.76
1:D:129:THR:HB	1:D:130:PRO:HD2	1.67	0.75
1:C:68:MET:CE	1:D:234:THR:HA	2.16	0.75
1:B:129:THR:HB	1:B:130:PRO:HD2	1.69	0.74
1:C:333:PRO:HG2	1:C:338:LEU:HD11	1.70	0.74
1:B:346:ARG:HD2	5:B:1540:HOH:O	1.87	0.73
1:A:129:THR:HB	1:A:130:PRO:HD2	1.71	0.73
1:B:147:MET:O	1:B:151:ARG:HG3	1.90	0.70
1:B:370:ARG:O	1:B:374:GLU:HG3	1.90	0.70
1:C:299:ARG:HA	5:C:1554:HOH:O	1.91	0.70
1:C:358:GLU:HB3	1:C:360:PRO:HD2	1.73	0.70
1:B:138:VAL:HG22	1:B:164:ASP:HB3	1.74	0.70
1:A:172:ARG:HB2	1:A:287:ASP:HB2	1.73	0.70
1:B:51:GLU:OE1	1:B:247:ARG:HD2	1.92	0.70
1:B:25:GLU:HG3	5:B:1342:HOH:O	1.91	0.70
1:C:300:ARG:HD3	1:C:348:VAL:O	1.91	0.69
1:B:224:ARG:HD2	1:B:230:GLU:OE1	1.91	0.69
1:C:299:ARG:HG2	1:C:299:ARG:NH1	2.02	0.69
1:A:68:MET:HE3	1:B:234:THR:HA	1.74	0.69
1:A:8:PRO:HD2	5:A:1595:HOH:O	1.94	0.68
1:D:15:LEU:CB	4:D:1310:EDO:H11	2.20	0.66
1:A:38:ARG:NH1	5:A:1483:HOH:O	2.29	0.66
1:A:234:THR:HA	1:B:68:MET:HE3	1.78	0.65
1:A:371:GLU:O	1:A:375:ARG:HG3	1.96	0.65
1:C:138:VAL:HG22	1:C:164:ASP:HB3	1.79	0.65
1:C:310:ARG:HH21	1:C:375:ARG:HH12	1.42	0.65
1:C:174:ARG:HG2	1:C:285:ASP:HB3	1.78	0.65
1:C:129:THR:HB	1:C:130:PRO:HD2	1.79	0.65
1:C:72:GLN:NE2	5:C:1626:HOH:O	2.28	0.64
1:C:76:ARG:HG2	5:C:1600:HOH:O	1.98	0.64
1:D:333:PRO:HG2	1:D:338:LEU:HD11	1.80	0.63
1:D:343:SER:O	1:D:347:GLN:HG3	1.98	0.63
1:B:299:ARG:NH2	1:B:302:GLU:OE1	2.30	0.62
1:A:234:THR:HA	1:B:68:MET:CE	2.29	0.62
1:D:359:ARG:HB3	1:D:360:PRO:HD3	1.81	0.61
1:A:84:ASP:HB3	1:A:133:ARG:HG3	1.82	0.61
1:B:125:GLU:OE1	1:B:156:ARG:NH1	2.34	0.61
1:B:169:HIS:CD2	1:B:169:HIS:H	2.19	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PHE:N	1:B:247:ARG:HD3	2.16	0.60
1:D:176:ARG:HH11	1:D:176:ARG:HG2	1.67	0.60
1:A:321:PRO:HG2	1:A:324:LEU:HD12	1.85	0.59
1:C:226:LYS:HD3	1:C:227:TYR:CE2	2.37	0.59
1:C:21:GLU:OE1	1:C:356:HIS:NE2	2.35	0.58
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.68	0.58
1:D:176:ARG:HB3	1:D:176:ARG:CZ	2.32	0.58
1:D:229:HIS:HD2	5:D:1323:HOH:O	1.86	0.58
1:A:152:GLU:OE2	1:A:156:ARG:NH2	2.37	0.57
1:A:315:LEU:CD2	1:B:226:LYS:HE2	2.34	0.57
1:D:89:PRO:HA	1:D:119:LEU:CD1	2.35	0.57
1:A:68:MET:CE	1:B:234:THR:HA	2.34	0.56
1:B:328:TYR:O	1:B:329:ALA:C	2.43	0.56
1:A:119:LEU:HD22	1:A:137:PRO:HA	1.87	0.56
1:C:332:ALA:HB1	1:C:333:PRO:HD2	1.87	0.56
1:A:51:GLU:OE1	1:A:247:ARG:HD2	2.05	0.56
1:B:153:LEU:O	1:B:157:HIS:HD2	1.89	0.56
1:B:229:HIS:HD2	5:B:1317:HOH:O	1.88	0.56
1:D:368:ALA:HA	1:D:371:GLU:HG2	1.88	0.56
1:A:129:THR:HB	1:A:130:PRO:CD	2.35	0.55
1:D:114:GLU:HB3	1:D:340:ARG:NH2	2.21	0.55
1:D:172:ARG:NH2	4:D:1311:EDO:O1	2.31	0.55
1:A:60:HIS:NE2	1:C:225:GLN:OE1	2.32	0.55
1:A:225:GLN:OE1	1:C:60:HIS:NE2	2.30	0.55
1:A:213:GLU:HG2	5:C:1419:HOH:O	2.08	0.54
1:A:138:VAL:HG22	1:A:164:ASP:HB3	1.89	0.54
1:C:327:ALA:O	1:D:232:LYS:NZ	2.39	0.54
1:A:359:ARG:O	1:A:363:LEU:HG	2.08	0.54
1:D:176:ARG:HH11	1:D:176:ARG:CG	2.21	0.53
1:A:283:ALA:HB1	1:A:284:PRO:HD2	1.90	0.53
1:D:225:GLN:HG2	1:D:228:SER:HB3	1.91	0.53
1:A:333:PRO:HG2	1:A:338:LEU:HD11	1.91	0.53
1:A:372:TRP:HA	1:A:375:ARG:HG3	1.90	0.53
1:C:227:TYR:HB3	1:D:319:PRO:HG2	1.91	0.53
1:C:129:THR:HB	1:C:130:PRO:CD	2.39	0.52
1:B:84:ASP:HB3	1:B:133:ARG:HG3	1.91	0.52
1:B:216:ARG:NH1	5:B:1600:HOH:O	2.37	0.52
1:D:129:THR:HB	1:D:130:PRO:CD	2.36	0.52
1:A:216:ARG:HD3	5:A:1394:HOH:O	2.10	0.52
1:A:241:MET:CE	1:B:241:MET:HE1	2.39	0.52
1:A:316:THR:HG23	1:A:348:VAL:O	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:HB2	1:A:318:TYR:CZ	2.45	0.52
1:D:87:ILE:HG23	1:D:110:VAL:HG23	1.91	0.52
1:D:89:PRO:HA	1:D:119:LEU:HD11	1.90	0.52
1:C:152:GLU:O	1:C:156:ARG:HG2	2.10	0.52
1:C:29:ALA:HB2	1:C:248:ILE:HD11	1.92	0.51
1:C:76:ARG:HD2	5:C:1364:HOH:O	2.09	0.51
1:D:329:ALA:HA	5:D:1458:HOH:O	2.10	0.51
1:C:299:ARG:HH11	1:C:299:ARG:CG	2.17	0.51
1:A:241:MET:HE3	1:B:241:MET:HE1	1.93	0.51
1:A:216:ARG:HB2	1:A:216:ARG:HH11	1.76	0.50
1:A:16:LYS:HE3	1:B:35:ASP:HA	1.93	0.50
1:C:169:HIS:H	1:C:169:HIS:CD2	2.29	0.50
1:A:221:TYR:CE2	1:B:68:MET:HE2	2.46	0.50
1:C:216:ARG:HD3	5:C:1421:HOH:O	2.10	0.50
1:A:68:MET:HE2	1:B:221:TYR:CE2	2.47	0.50
1:A:221:TYR:CE2	1:B:95:ALA:HB2	2.46	0.50
1:A:359:ARG:HB3	1:A:360:PRO:HD3	1.94	0.50
1:B:284:PRO:O	1:B:285:ASP:HB2	2.12	0.50
1:B:307:LEU:HD12	1:B:314:THR:HG21	1.93	0.50
1:D:298:GLU:O	1:D:299:ARG:HB2	2.10	0.50
1:C:227:TYR:CD1	1:D:319:PRO:HG3	2.47	0.50
1:B:48:PHE:CA	1:B:247:ARG:HD3	2.42	0.49
1:C:298:GLU:HG2	1:C:347:GLN:HE21	1.78	0.49
1:A:220:ASN:O	1:A:221:TYR:HB2	2.12	0.49
1:C:300:ARG:O	1:C:300:ARG:HG2	2.01	0.49
1:D:220:ASN:O	1:D:221:TYR:HB2	2.12	0.49
1:A:226:LYS:O	1:A:227:TYR:HB2	2.13	0.48
1:A:229:HIS:HE1	4:A:1304:EDO:O2	1.96	0.48
1:C:193:LLP:OP3	1:D:221:TYR:OH	2.30	0.48
1:B:21:GLU:OE1	1:B:356:HIS:NE2	2.41	0.48
1:D:15:LEU:H	4:D:1310:EDO:C2	2.27	0.48
1:D:129:THR:CB	1:D:130:PRO:HD2	2.42	0.48
1:B:220:ASN:O	1:B:221:TYR:HB2	2.14	0.48
1:D:306:HIS:O	1:D:310:ARG:HG2	2.14	0.48
1:A:21:GLU:O	1:A:22:LEU:HD23	2.13	0.48
1:A:332:ALA:HB1	1:A:333:PRO:HD2	1.96	0.48
1:A:358:GLU:O	1:A:361:GLN:HB2	2.14	0.47
1:A:154:ALA:HB2	1:A:161:ILE:HD11	1.95	0.47
1:D:133:ARG:HA	1:D:133:ARG:HD3	1.50	0.47
1:A:128:ILE:HD13	1:A:159:LEU:HD11	1.96	0.47
1:D:358:GLU:HB3	1:D:360:PRO:HD2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:MET:CE	1:B:242:GLN:NE2	2.78	0.47
1:B:328:TYR:O	1:B:330:GLY:N	2.48	0.47
1:D:89:PRO:HB3	1:D:119:LEU:HD13	1.96	0.47
1:D:243:ALA:O	1:D:247:ARG:HG3	2.14	0.47
1:A:8:PRO:O	1:A:364:ARG:NH1	2.32	0.47
1:D:361:GLN:O	1:D:365:VAL:HG23	2.15	0.47
1:A:241:MET:HE1	1:B:242:GLN:NE2	2.29	0.47
1:D:9:ARG:NH2	1:D:308:ASP:OD1	2.48	0.47
1:A:193:LLP:OP3	1:B:221:TYR:OH	2.29	0.47
1:A:221:TYR:CE2	1:B:68:MET:CE	2.97	0.47
1:A:227:TYR:H	4:A:1304:EDO:C1	2.27	0.46
1:C:227:TYR:CE2	4:C:1309:EDO:H11	2.50	0.46
1:A:193:LLP:NZ	1:A:193:LLP:O3	2.48	0.46
1:A:97:TRP:CD2	1:A:322:VAL:HG11	2.50	0.46
1:B:208:ASP:HA	1:B:209:PRO:HD3	1.82	0.46
1:A:135:LEU:HB2	1:A:161:ILE:HG12	1.97	0.46
1:B:359:ARG:N	1:B:360:PRO:HD2	2.29	0.46
1:D:92:THR:OG1	1:D:93:TYR:N	2.48	0.46
1:A:237:ARG:NH2	1:B:200:ASP:OD1	2.42	0.46
1:C:148:ASP:HB2	1:C:174:ARG:NH1	2.30	0.46
1:C:226:LYS:HG3	1:C:227:TYR:N	2.30	0.46
1:B:226:LYS:HE3	4:B:1304:EDO:O1	2.15	0.46
1:A:68:MET:CE	1:B:221:TYR:CE2	2.99	0.46
1:A:229:HIS:HD2	5:A:1548:HOH:O	1.99	0.46
1:B:217:MET:HE3	1:B:224:ARG:HG2	1.96	0.46
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.80	0.46
1:B:359:ARG:HB3	1:B:360:PRO:HD3	1.97	0.46
1:D:97:TRP:CD2	1:D:322:VAL:HG11	2.50	0.46
1:A:89:PRO:HB3	1:A:119:LEU:HD13	1.97	0.45
1:B:9:ARG:NH1	1:B:311:GLY:HA2	2.32	0.45
1:B:153:LEU:CD1	1:B:156:ARG:NH1	2.80	0.45
1:B:361:GLN:HG3	5:B:1444:HOH:O	2.15	0.45
1:C:28:ALA:HA	4:C:1308:EDO:O1	2.16	0.45
1:D:138:VAL:HG22	1:D:164:ASP:HB3	1.98	0.45
1:C:376:VAL:HG21	5:C:1619:HOH:O	2.16	0.45
1:D:371:GLU:O	1:D:375:ARG:HB2	2.16	0.45
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.77	0.45
1:D:193:LLP:O3	1:D:193:LLP:NZ	2.49	0.45
1:A:282:THR:HG23	1:A:288:PRO:HG3	1.99	0.45
1:D:111:GLU:HB3	1:D:112:PRO:HD2	1.99	0.45
1:A:302:GLU:HG3	5:A:1573:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:HD13	5:D:1522:HOH:O	2.16	0.45
1:B:333:PRO:HG2	1:B:338:LEU:HD11	1.99	0.45
1:C:68:MET:CE	1:D:221:TYR:CE2	2.99	0.45
1:B:222:GLY:HA3	1:B:231:THR:O	2.17	0.45
1:D:88:VAL:O	1:D:109:PRO:HA	2.17	0.45
1:D:332:ALA:HB1	1:D:333:PRO:HD2	1.98	0.45
1:B:299:ARG:HA	5:B:1586:HOH:O	2.18	0.44
1:B:9:ARG:HB3	1:B:311:GLY:O	2.17	0.44
1:C:300:ARG:HG3	1:C:349:LEU:HB2	2.00	0.43
1:A:333:PRO:HB2	1:A:337:SER:OG	2.17	0.43
1:B:30:ILE:O	1:B:34:LEU:HG	2.18	0.43
1:C:78:LEU:HB2	1:C:80:ILE:HD12	1.99	0.43
1:A:291:HIS:CD2	1:A:292:LEU:HG	2.53	0.43
1:B:359:ARG:N	1:B:360:PRO:CD	2.82	0.43
1:A:194:ASN:OD1	1:A:291:HIS:HA	2.18	0.43
1:C:33:VAL:HG22	1:C:44:GLU:HG3	2.00	0.43
1:C:243:ALA:O	1:C:247:ARG:HG3	2.18	0.43
1:D:208:ASP:HA	1:D:209:PRO:HD2	1.89	0.43
1:A:334:PRO:O	1:A:335:GLU:C	2.55	0.43
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.84	0.43
1:C:307:LEU:HD12	1:C:314:THR:HG21	2.00	0.43
1:C:321:PRO:HB2	1:C:323:HIS:CE1	2.53	0.43
1:A:357:LEU:HD11	1:A:361:GLN:HB3	2.01	0.43
1:C:72:GLN:HG3	1:C:103:THR:HG22	2.01	0.43
1:D:371:GLU:HG3	1:D:372:TRP:N	2.34	0.43
1:B:234:THR:OG1	1:B:235:ASN:N	2.52	0.43
1:C:321:PRO:HG2	1:C:324:LEU:HD12	2.00	0.43
1:B:129:THR:HB	1:B:130:PRO:CD	2.41	0.42
1:D:89:PRO:CB	1:D:119:LEU:HD13	2.49	0.42
1:C:310:ARG:NH2	1:C:375:ARG:HH12	2.12	0.42
1:D:176:ARG:CG	1:D:176:ARG:NH1	2.80	0.42
1:D:283:ALA:HB1	1:D:284:PRO:HD2	2.01	0.42
1:A:366:ILE:O	1:A:370:ARG:HB2	2.20	0.42
1:A:84:ASP:CB	1:A:133:ARG:HG3	2.47	0.42
1:A:144:PRO:HB3	1:A:178:ILE:HD11	2.01	0.42
1:A:363:LEU:HD23	1:A:366:ILE:HD12	2.01	0.42
1:A:193:LLP:OP2	4:A:1305:EDO:O2	2.38	0.42
1:B:124:VAL:HB	1:B:153:LEU:HD21	2.02	0.42
1:C:126:LYS:HB3	1:C:126:LYS:HE2	1.83	0.42
1:D:142:GLY:HA2	1:D:167:GLN:O	2.20	0.42
1:D:191:PRO:O	4:D:1308:EDO:H21	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:SER:O	1:D:206:THR:HA	2.19	0.41
1:A:241:MET:CE	1:B:242:GLN:HE22	2.32	0.41
1:D:78:LEU:HD23	1:D:78:LEU:HA	1.88	0.41
1:B:310:ARG:HD2	1:B:371:GLU:OE2	2.20	0.41
1:C:221:TYR:OH	1:D:193:LLP:OP3	2.37	0.41
1:A:151:ARG:HH11	1:A:151:ARG:HD2	1.75	0.41
1:D:321:PRO:HB2	1:D:323:HIS:CE1	2.55	0.41
1:A:55:TYR:O	4:A:1301:EDO:O2	2.39	0.41
1:B:298:GLU:OE1	1:B:298:GLU:HA	2.21	0.41
1:C:300:ARG:HD3	1:C:300:ARG:HH11	1.51	0.41
1:D:22:LEU:HD13	1:D:248:ILE:HG22	2.01	0.41
1:D:171:ALA:HB2	1:D:289:VAL:HG22	2.01	0.41
1:C:227:TYR:CD2	4:C:1309:EDO:H11	2.56	0.41
1:C:291:HIS:CD2	1:C:292:LEU:HG	2.56	0.41
1:D:323:HIS:CE1	1:D:342:GLU:HG3	2.56	0.41
1:B:190:TYR:CD1	1:B:191:PRO:HD2	2.55	0.41
1:B:226:LYS:O	1:B:227:TYR:HB2	2.21	0.41
1:C:193:LLP:O3	1:C:193:LLP:NZ	2.54	0.41
1:D:87:ILE:HG23	1:D:110:VAL:CG2	2.50	0.41
1:A:126:LYS:HE3	1:A:126:LYS:HB3	1.71	0.41
1:B:173:TYR:CE2	1:B:174:ARG:HG3	2.55	0.41
1:B:298:GLU:O	1:B:299:ARG:HB2	2.21	0.41
1:C:88:VAL:O	1:C:109:PRO:HA	2.21	0.41
1:D:226:LYS:O	1:D:227:TYR:HB2	2.20	0.41
1:A:190:TYR:CD1	1:A:191:PRO:HD2	2.56	0.41
1:B:172:ARG:HA	1:B:176:ARG:O	2.20	0.41
1:B:252:HIS:HD2	5:B:1461:HOH:O	2.03	0.41
1:A:241:MET:HE3	1:A:241:MET:HB3	1.74	0.40
1:C:97:TRP:CD2	1:C:322:VAL:HG11	2.55	0.40
1:D:126:LYS:HB3	1:D:126:LYS:HE2	1.47	0.40
1:C:142:GLY:HA2	1:C:167:GLN:O	2.21	0.40
1:A:58:THR:HG21	1:A:205:VAL:HB	2.04	0.40
1:C:226:LYS:HG3	1:C:227:TYR:CD2	2.55	0.40
1:A:241:MET:CE	1:B:241:MET:CE	2.99	0.40
1:C:131:ARG:HG2	1:C:131:ARG:NH1	2.33	0.40
1:C:216:ARG:NH2	5:C:1611:HOH:O	2.39	0.40
1:D:48:PHE:CE1	1:D:246:LEU:HB3	2.57	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	365/399 (92%)	350 (96%)	15 (4%)	0	100	100
1	B	366/399 (92%)	351 (96%)	14 (4%)	1 (0%)	41	31
1	C	366/399 (92%)	347 (95%)	18 (5%)	1 (0%)	41	31
1	D	365/399 (92%)	351 (96%)	13 (4%)	1 (0%)	41	31
All	All	1462/1596 (92%)	1399 (96%)	60 (4%)	3 (0%)	47	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	ALA
1	D	299	ARG
1	C	117	PRO

### 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	287/314 (91%)	274 (96%)	13 (4%)	27	20
1	B	288/314 (92%)	277 (96%)	11 (4%)	33	26
1	C	288/314 (92%)	282 (98%)	6 (2%)	53	48
1	D	287/314 (91%)	273 (95%)	14 (5%)	25	17
All	All	1150/1256 (92%)	1106 (96%)	44 (4%)	33	26

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	126	LYS
1	A	153	LEU
1	A	156	ARG
1	A	174	ARG
1	A	241	MET
1	A	255	SER
1	A	285	ASP
1	A	299	ARG
1	A	305	SER
1	A	331	GLU
1	A	344	PHE
1	A	346	ARG
1	B	35	ASP
1	B	38	ARG
1	B	152	GLU
1	B	156	ARG
1	B	174	ARG
1	B	224	ARG
1	B	284	PRO
1	B	300	ARG
1	B	305	SER
1	B	331	GLU
1	B	350	SER
1	C	25	GLU
1	C	38	ARG
1	C	68	MET
1	C	241	MET
1	C	299	ARG
1	C	358	GLU
1	D	38	ARG
1	D	68	MET
1	D	121	PRO
1	D	126	LYS
1	D	133	ARG
1	D	153	LEU
1	D	176	ARG
1	D	225	GLN
1	D	226	LYS
1	D	285	ASP
1	D	344	PHE
1	D	346	ARG
1	D	348	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	359	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	157	HIS
1	A	229	HIS
1	B	72	GLN
1	B	157	HIS
1	B	169	HIS
1	B	229	HIS
1	C	169	HIS
1	C	306	HIS
1	D	72	GLN
1	D	157	HIS
1	D	229	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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
1	LLP	A	193	1	23,24,25	1.42	2 (8%)	25,32,34	0.96	0
1	LLP	B	193	1	23,24,25	1.45	3 (13%)	25,32,34	0.98	0
1	LLP	D	193	1	23,24,25	1.28	2 (8%)	25,32,34	0.92	0
1	LLP	C	193	1	23,24,25	1.37	2 (8%)	25,32,34	0.99	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
1	LLP	A	193	1	-	1/16/17/19	0/1/1/1
1	LLP	B	193	1	-	3/16/17/19	0/1/1/1
1	LLP	D	193	1	-	2/16/17/19	0/1/1/1
1	LLP	C	193	1	-	2/16/17/19	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	LLP	C4'-NZ	5.31	1.45	1.27
1	B	193	LLP	C4'-NZ	4.57	1.42	1.27
1	C	193	LLP	C4'-NZ	4.57	1.42	1.27
1	D	193	LLP	C4'-NZ	3.90	1.40	1.27
1	D	193	LLP	P-OP1	3.09	1.60	1.50
1	A	193	LLP	P-OP1	2.85	1.59	1.50
1	C	193	LLP	P-OP1	2.66	1.59	1.50
1	B	193	LLP	C3-C2	-2.62	1.38	1.40
1	B	193	LLP	P-OP1	2.60	1.58	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	193	LLP	CG-CD-CE-NZ
1	D	193	LLP	C4-C4'-NZ-CE
1	B	193	LLP	CG-CD-CE-NZ
1	C	193	LLP	CG-CD-CE-NZ
1	D	193	LLP	CG-CD-CE-NZ
1	B	193	LLP	CD-CE-NZ-C4'
1	C	193	LLP	C4-C4'-NZ-CE
1	B	193	LLP	C4-C4'-NZ-CE

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	193	LLP	3	0
1	D	193	LLP	2	0
1	C	193	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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	EDO	A	1302	-	3,3,3	1.14	0	2,2,2	0.43	0
4	EDO	A	1301	-	3,3,3	1.21	0	2,2,2	0.24	0
4	EDO	A	1306	-	3,3,3	1.08	0	2,2,2	0.44	0
4	EDO	C	1307	-	3,3,3	1.13	0	2,2,2	0.37	0
4	EDO	C	1308	-	3,3,3	1.19	0	2,2,2	0.45	0
4	EDO	D	1310	-	3,3,3	1.09	0	2,2,2	0.40	0
4	EDO	D	1311	-	3,3,3	1.22	0	2,2,2	0.30	0
4	EDO	B	1302	-	3,3,3	1.08	0	2,2,2	0.39	0
4	EDO	D	1312	-	3,3,3	1.11	0	2,2,2	0.38	0
4	EDO	D	1308	-	3,3,3	1.11	0	2,2,2	0.30	0
4	EDO	B	1304	-	3,3,3	1.05	0	2,2,2	0.40	0
4	EDO	D	1307	-	3,3,3	1.09	0	2,2,2	0.48	0
4	EDO	A	1300	-	3,3,3	1.06	0	2,2,2	0.43	0
4	EDO	C	1305	-	3,3,3	1.15	0	2,2,2	0.41	0
4	EDO	C	1309	-	3,3,3	1.12	0	2,2,2	0.49	0
4	EDO	A	1304	-	3,3,3	1.12	0	2,2,2	0.35	0
4	EDO	B	1303	-	3,3,3	1.10	0	2,2,2	0.39	0
4	EDO	C	1306	-	3,3,3	1.12	0	2,2,2	0.40	0
4	EDO	A	1303	-	3,3,3	1.13	0	2,2,2	0.40	0
4	EDO	A	1305	-	3,3,3	1.06	0	2,2,2	0.37	0
4	EDO	D	1309	-	3,3,3	1.10	0	2,2,2	0.53	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	A	1302	-	-	0/1/1/1	-
4	EDO	A	1301	-	-	1/1/1/1	-
4	EDO	A	1306	-	-	1/1/1/1	-
4	EDO	C	1307	-	-	1/1/1/1	-
4	EDO	C	1308	-	-	1/1/1/1	-
4	EDO	D	1310	-	-	0/1/1/1	-
4	EDO	D	1311	-	-	1/1/1/1	-
4	EDO	B	1302	-	-	0/1/1/1	-
4	EDO	D	1312	-	-	1/1/1/1	-
4	EDO	D	1308	-	-	0/1/1/1	-
4	EDO	B	1304	-	-	1/1/1/1	-
4	EDO	D	1307	-	-	0/1/1/1	-
4	EDO	A	1300	-	-	0/1/1/1	-
4	EDO	C	1305	-	-	1/1/1/1	-
4	EDO	C	1309	-	-	1/1/1/1	-
4	EDO	A	1304	-	-	1/1/1/1	-
4	EDO	B	1303	-	-	0/1/1/1	-
4	EDO	C	1306	-	-	0/1/1/1	-
4	EDO	A	1303	-	-	0/1/1/1	-
4	EDO	A	1305	-	-	0/1/1/1	-
4	EDO	D	1309	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	EDO	O1-C1-C2-O2
4	D	1311	EDO	O1-C1-C2-O2
4	A	1306	EDO	O1-C1-C2-O2
4	B	1304	EDO	O1-C1-C2-O2
4	C	1307	EDO	O1-C1-C2-O2
4	C	1308	EDO	O1-C1-C2-O2
4	C	1309	EDO	O1-C1-C2-O2
4	D	1312	EDO	O1-C1-C2-O2
4	C	1305	EDO	O1-C1-C2-O2
4	A	1304	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	EDO	1	0
4	C	1308	EDO	1	0
4	D	1310	EDO	3	0
4	D	1311	EDO	1	0
4	D	1308	EDO	1	0
4	B	1304	EDO	1	0
4	C	1309	EDO	2	0
4	A	1304	EDO	2	0
4	A	1305	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	367/399 (91%)	-0.43	2 (0%) 91 92	11, 20, 44, 81	0
1	B	368/399 (92%)	-0.48	3 (0%) 86 88	10, 20, 46, 80	0
1	C	368/399 (92%)	-0.53	4 (1%) 80 82	10, 18, 43, 77	0
1	D	367/399 (91%)	-0.42	4 (1%) 80 82	11, 21, 48, 95	0
All	All	1470/1596 (92%)	-0.46	13 (0%) 84 86	10, 20, 46, 95	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	375	ARG	5.3
1	B	376	VAL	4.3
1	B	375	ARG	3.3
1	C	375	ARG	3.2
1	D	130	PRO	2.9
1	C	376	VAL	2.6
1	B	130	PRO	2.6
1	A	375	ARG	2.4
1	A	156	ARG	2.3
1	C	156	ARG	2.1
1	C	275	PRO	2.1
1	D	156	ARG	2.1
1	D	334	PRO	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. 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( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	193	24/25	0.97	0.12	10,16,26,54	0
1	LLP	C	193	24/25	0.97	0.12	5,14,21,37	0
1	LLP	B	193	24/25	0.98	0.11	5,15,22,38	0
1	LLP	D	193	24/25	0.98	0.12	8,14,22,41	0

### 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( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	1309	4/4	0.73	0.27	34,51,61,90	0
4	EDO	B	1304	4/4	0.78	0.24	51,58,64,88	0
4	EDO	A	1306	4/4	0.83	0.28	43,47,100,100	0
4	EDO	D	1311	4/4	0.83	0.22	43,51,83,100	0
4	EDO	C	1307	4/4	0.87	0.18	37,45,55,67	0
4	EDO	C	1308	4/4	0.88	0.18	38,52,60,62	0
4	EDO	A	1304	4/4	0.90	0.17	26,36,56,100	0
4	EDO	C	1305	4/4	0.90	0.18	29,34,39,76	0
4	EDO	D	1310	4/4	0.91	0.24	13,32,45,78	0
4	EDO	A	1305	4/4	0.91	0.15	30,34,44,49	0
4	EDO	A	1300	4/4	0.92	0.18	38,39,39,43	0
4	EDO	B	1302	4/4	0.93	0.17	27,36,43,45	0
4	EDO	D	1312	4/4	0.93	0.20	26,33,41,51	0
4	EDO	D	1309	4/4	0.94	0.13	21,37,40,42	0
4	EDO	A	1302	4/4	0.94	0.13	27,34,52,54	0
4	EDO	A	1301	4/4	0.94	0.12	24,37,41,44	0
4	EDO	D	1307	4/4	0.94	0.13	25,30,32,33	0
4	EDO	D	1308	4/4	0.95	0.11	20,20,21,28	0
4	EDO	C	1306	4/4	0.96	0.11	24,31,33,43	0
4	EDO	A	1303	4/4	0.97	0.11	21,23,28,32	0
4	EDO	B	1303	4/4	0.97	0.10	22,23,28,29	0
2	CL	B	1301	1/1	0.98	0.06	38,38,38,38	0
2	CL	C	1303	1/1	0.98	0.06	30,30,30,30	0
2	CL	D	1305	1/1	0.98	0.07	27,27,27,27	0
3	NA	A	1299	1/1	0.98	0.17	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	1297	1/1	0.98	0.04	30,30,30,30	0
3	NA	C	1304	1/1	0.99	0.20	12,12,12,12	0
2	CL	A	1298	1/1	0.99	0.08	22,22,22,22	0
2	CL	D	1306	1/1	1.00	0.06	23,23,23,23	0
2	CL	B	1300	1/1	1.00	0.05	27,27,27,27	0
2	CL	C	1302	1/1	1.00	0.04	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.