



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:29 PM GMT

PDB ID : 2C7F
Title : THE STRUCTURE OF A FAMILY 51 ARABINOFURANOSIDASE, ARAF51, FROM CLOSTRIDIUM THERMOCELLUM IN COMPLEX WITH 1,5-ALPHA-L-ARABINOTRIOSE.
Authors : Taylor, E.J.; Smith, N.L.; Turkenburg, J.P.; D'Souza, S.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-11-23
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

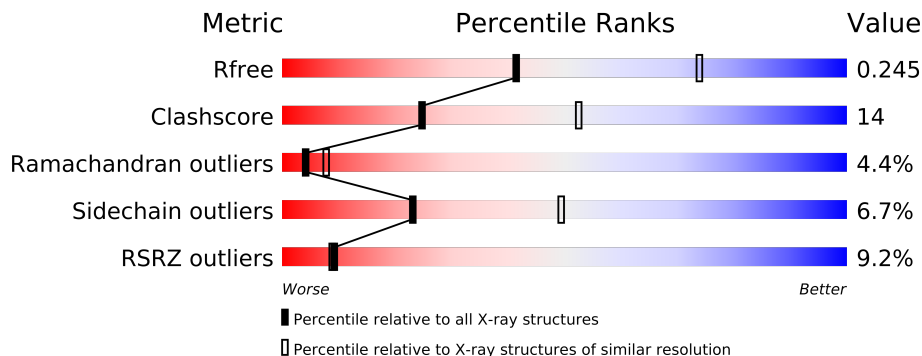
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	513	
1	B	513	
1	C	513	
1	D	513	
1	E	513	
1	F	513	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	B	1505	-	X
3	EDO	D	1506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	D	1507	-	X
3	EDO	E	1506	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24046 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ALPHA-L-ARABINOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3971	2523	676	750	22			
1	B	497	Total	C	N	O	S	0	0	0
			3972	2518	680	753	21			
1	C	496	Total	C	N	O	S	0	1	0
			3977	2523	679	753	22			
1	D	499	Total	C	N	O	S	0	0	0
			3978	2522	680	754	22			
1	E	492	Total	C	N	O	S	0	0	1
			3886	2465	663	738	20			
1	F	496	Total	C	N	O	S	0	0	0
			3959	2513	674	751	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
B	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
C	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
D	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
E	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
F	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			28	15	13		
2	C	3	Total	C	O	0	0
			28	15	13		
2	D	3	Total	C	O	0	0
			28	15	13		

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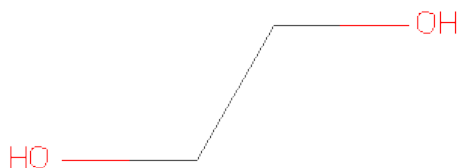
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	3	Total	C	O	0	0
			28	15	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
C	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
D	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
E	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	2	Total	C	O	0	0
			19	10	9		
4	F	2	Total	C	O	0	0
			19	10	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5
F	173	ALA	GLU	ENGINEERED MUTATION	UNP Q4CJG5

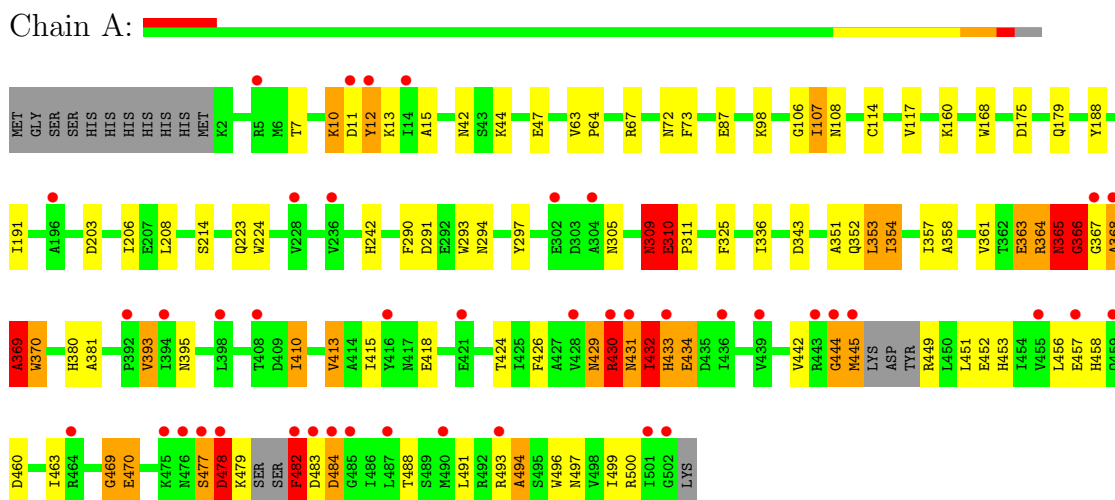
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	17	Total	O	0	0
			17	17		
5	C	19	Total	O	0	0
			19	19		
5	D	21	Total	O	0	0
			21	21		
5	E	15	Total	O	0	0
			15	15		
5	F	19	Total	O	0	0
			19	19		

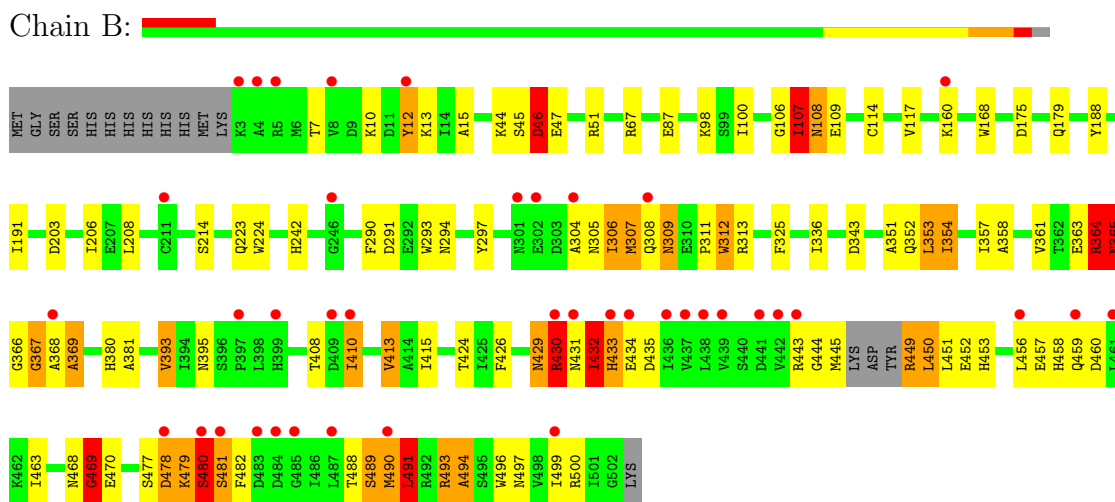
3 Residue-property plots

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.

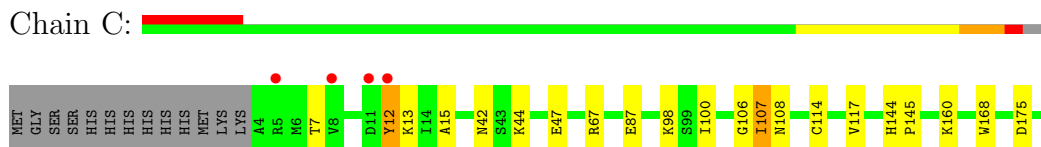
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

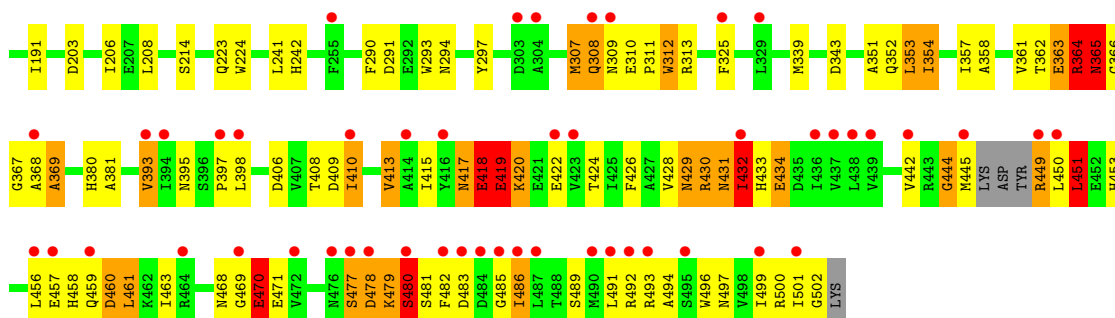


• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE



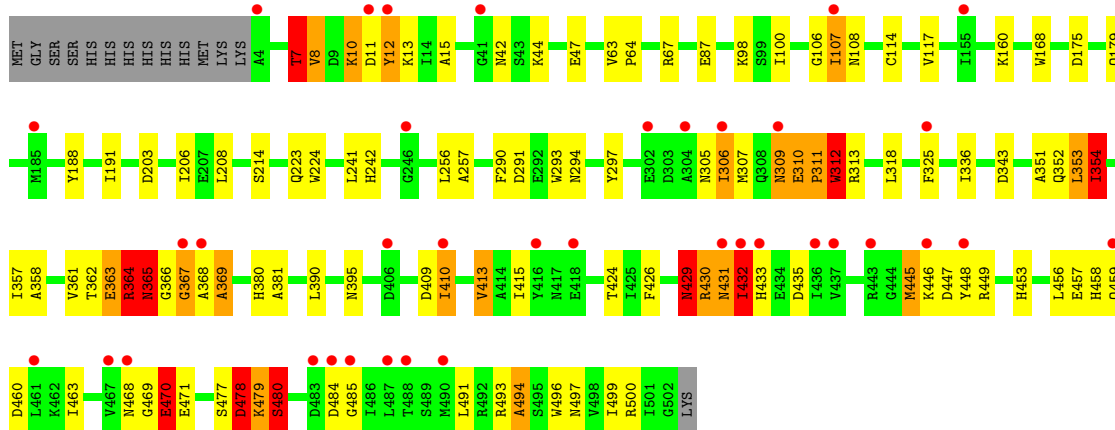
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE





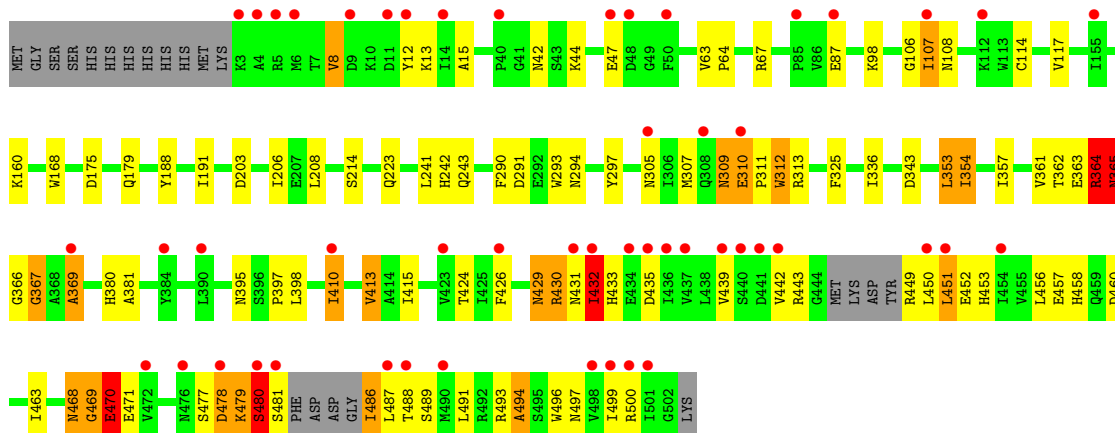
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

Chain D:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

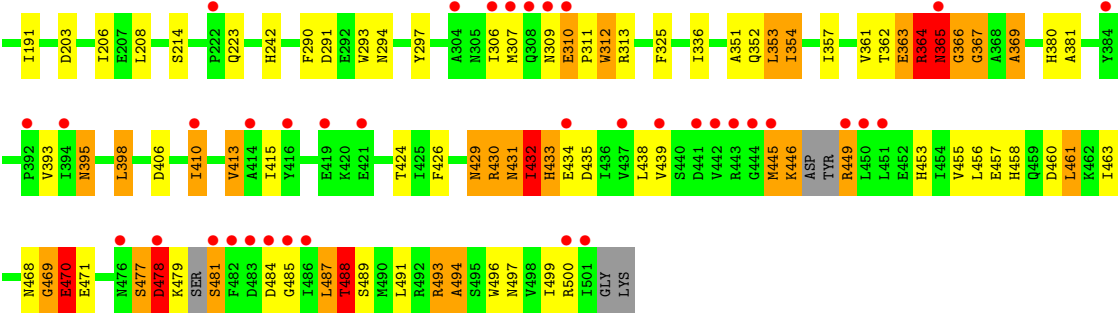
Chain E:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.34Å 173.34Å 272.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.86 – 2.70 59.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (145.86-2.70) 99.7 (59.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.255 0.231 , 0.245	Depositor DCC
R_{free} test set	5684 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 17.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113743 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24046	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4061	0.57	1/5499 (0.0%)
1	B	0.36	0/4063	0.59	2/5503 (0.0%)
1	C	0.36	0/4068	0.58	0/5514
1	D	0.34	0/4071	0.57	1/5516 (0.0%)
1	E	0.33	0/3973	0.55	0/5382
1	F	0.32	0/4049	0.55	1/5485 (0.0%)
All	All	0.34	0/24285	0.57	5/32899 (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	18
1	B	0	20
1	C	0	17
1	D	0	15
1	E	0	11
1	F	1	17
All	All	1	98

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	N-CA-C	6.22	127.80	111.00
1	F	461	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	310	GLU	N-CA-C	5.37	125.50	111.00
1	B	491	LEU	CA-CB-CG	5.25	127.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	LEU	CB-CG-CD2	5.05	119.59	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	479	LYS	CA

All (98) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLN	Peptide
1	A	309	ASN	Peptide
1	A	353	LEU	Peptide
1	A	365	ASN	Peptide
1	A	366	GLY	Peptide
1	A	367	GLY	Peptide
1	A	368	ALA	Peptide
1	A	369	ALA	Peptide
1	A	393	VAL	Peptide
1	A	429	ASN	Peptide
1	A	430	ARG	Peptide
1	A	431	ASN	Peptide
1	A	433	HIS	Peptide
1	A	444	GLY	Peptide
1	A	469	GLY	Peptide
1	A	478	ASP	Peptide
1	A	482	PHE	Peptide
1	A	72	ASN	Peptide
1	B	107	ILE	Peptide
1	B	109	GLU	Peptide
1	B	223	GLN	Peptide
1	B	304	ALA	Peptide
1	B	306	ILE	Peptide
1	B	307	MET	Peptide
1	B	309	ASN	Peptide
1	B	312	TRP	Peptide
1	B	353	LEU	Peptide
1	B	365	ASN	Peptide
1	B	366	GLY	Peptide
1	B	367	GLY	Peptide
1	B	429	ASN	Peptide
1	B	430	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	432	ILE	Peptide
1	B	444	GLY	Peptide
1	B	45	SER	Peptide
1	B	469	GLY	Peptide
1	B	489	SER	Peptide
1	B	491	LEU	Peptide
1	C	223	GLN	Peptide
1	C	307	MET	Peptide
1	C	312	TRP	Peptide
1	C	353	LEU	Peptide
1	C	364	ARG	Peptide
1	C	365	ASN	Peptide
1	C	367	GLY	Peptide
1	C	417	ASN	Peptide
1	C	418	GLU	Peptide
1	C	419	GLU	Peptide
1	C	429	ASN	Peptide
1	C	431	ASN	Peptide
1	C	444	GLY	Peptide
1	C	450	LEU	Peptide
1	C	460	ASP	Peptide
1	C	470	GLU	Peptide
1	C	471	GLU	Peptide
1	D	223	GLN	Peptide
1	D	307	MET	Peptide
1	D	309	ASN	Peptide
1	D	311	PRO	Peptide
1	D	312	TRP	Peptide
1	D	353	LEU	Peptide
1	D	364	ARG	Peptide
1	D	365	ASN	Peptide
1	D	367	GLY	Peptide
1	D	429	ASN	Peptide
1	D	431	ASN	Peptide
1	D	471	GLU	Peptide
1	D	478	ASP	Peptide
1	D	480	SER	Peptide
1	D	7	THR	Peptide
1	E	223	GLN	Peptide
1	E	307	MET	Peptide
1	E	312	TRP	Peptide
1	E	353	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	E	364	ARG	Peptide
1	E	367	GLY	Peptide
1	E	429	ASN	Peptide
1	E	430	ARG	Peptide
1	E	443	ARG	Peptide
1	E	471	GLU	Peptide
1	E	480	SER	Peptide
1	F	223	GLN	Peptide
1	F	307	MET	Peptide
1	F	312	TRP	Peptide
1	F	353	LEU	Peptide
1	F	364	ARG	Peptide
1	F	365	ASN	Peptide
1	F	366	GLY	Peptide
1	F	367	GLY	Peptide
1	F	4	ALA	Peptide
1	F	429	ASN	Peptide
1	F	431	ASN	Peptide
1	F	445	MET	Peptide
1	F	471	GLU	Peptide
1	F	477	SER	Peptide
1	F	478	ASP	Peptide
1	F	487	LEU	Peptide
1	F	488	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3971	0	3869	112	0
1	B	3972	0	3852	113	0
1	C	3977	0	3857	123	0
1	D	3978	0	3854	111	0
1	E	3886	0	3756	98	0
1	F	3959	0	3834	106	0
2	A	28	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	21	0	0
2	D	28	0	21	1	0
2	E	28	0	21	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	E	8	0	12	0	0
3	F	4	0	6	0	0
4	B	19	0	15	0	0
4	F	19	0	15	0	0
5	A	26	0	0	0	0
5	B	17	0	0	0	0
5	C	19	0	0	0	0
5	D	21	0	0	0	0
5	E	15	0	0	1	0
5	F	19	0	0	0	0
All	All	24046	0	23190	654	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (654) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:478:ASP:CB	1:C:479:LYS:HB2	1.30	1.62
1:A:431:ASN:HA	1:A:432:ILE:CG2	1.39	1.53
1:E:431:ASN:CB	1:E:432:ILE:HG22	1.35	1.52
1:C:478:ASP:HB3	1:C:479:LYS:CB	1.46	1.45
1:A:431:ASN:CA	1:A:432:ILE:HG22	1.43	1.43
1:C:478:ASP:CA	1:C:479:LYS:HB2	1.50	1.35
1:B:450:LEU:HD12	1:B:451:LEU:N	1.48	1.26
1:F:445:MET:CA	1:F:446:LYS:HB2	1.61	1.25
1:E:431:ASN:HA	1:E:432:ILE:CB	1.62	1.23
1:A:478:ASP:CB	1:A:479:LYS:HB3	1.70	1.22
1:D:429:ASN:HA	1:D:430:ARG:CB	1.70	1.22
1:F:477:SER:HB2	1:F:478:ASP:OD1	1.42	1.19
1:F:4:ALA:HB1	1:F:5:ARG:CB	1.72	1.18
1:B:450:LEU:C	1:B:450:LEU:HD12	1.52	1.18
1:C:478:ASP:CB	1:C:479:LYS:CB	2.10	1.18
1:E:431:ASN:CA	1:E:432:ILE:HB	1.72	1.18
1:E:431:ASN:CB	1:E:432:ILE:CG2	2.23	1.17
1:E:432:ILE:H	1:E:493:ARG:HB2	1.09	1.15

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:478:ASP:HB3	1:A:479:LYS:HB3	1.15	1.13
1:E:431:ASN:HB2	1:E:432:ILE:HG22	1.27	1.12
1:F:445:MET:HA	1:F:446:LYS:HB2	1.12	1.12
1:B:469:GLY:HA2	1:B:470:GLU:HB2	1.21	1.11
1:B:449:ARG:HH11	1:B:449:ARG:HG2	1.07	1.10
1:E:429:ASN:O	1:E:431:ASN:O	1.67	1.10
1:B:469:GLY:HA2	1:B:470:GLU:CB	1.81	1.09
1:F:4:ALA:CB	1:F:5:ARG:CB	2.30	1.09
1:B:107:ILE:HG13	1:B:108:ASN:H	1.10	1.08
1:D:429:ASN:HA	1:D:430:ARG:HB3	1.27	1.08
1:C:418:GLU:HG3	1:C:419:GLU:CB	1.83	1.07
1:D:409:ASP:O	1:D:429:ASN:HB2	1.54	1.07
1:F:478:ASP:HB3	1:F:479:LYS:HA	1.26	1.07
1:B:449:ARG:HH11	1:B:449:ARG:CG	1.67	1.07
1:F:477:SER:CB	1:F:478:ASP:OD1	2.02	1.07
1:C:418:GLU:CG	1:C:419:GLU:HB3	1.85	1.06
1:E:431:ASN:HB3	1:E:432:ILE:CG2	1.82	1.05
1:A:478:ASP:HA	1:A:479:LYS:HB2	1.36	1.05
1:A:444:GLY:CA	1:A:445:MET:HB2	1.88	1.04
1:B:490:MET:O	1:B:491:LEU:HD23	1.56	1.03
1:F:4:ALA:CA	1:F:5:ARG:CB	2.37	1.03
1:D:431:ASN:HA	1:D:432:ILE:HG22	1.37	1.02
1:C:444:GLY:HA3	1:C:445:MET:HB2	1.40	1.02
1:E:431:ASN:HB3	1:E:432:ILE:HG22	1.07	1.02
1:A:444:GLY:HA3	1:A:445:MET:HB2	1.40	1.00
1:C:485:GLY:HA2	1:C:486:ILE:O	1.59	1.00
1:F:445:MET:CB	1:F:446:LYS:HB2	1.91	1.00
1:B:450:LEU:CD1	1:B:450:LEU:C	2.30	0.99
1:A:478:ASP:HB3	1:A:479:LYS:CB	1.92	0.99
1:C:478:ASP:HB3	1:C:479:LYS:HB3	1.38	0.99
1:C:478:ASP:HA	1:C:479:LYS:HB2	1.40	0.98
1:A:442:VAL:HG22	1:A:445:MET:HB3	1.45	0.97
1:B:107:ILE:HG13	1:B:108:ASN:N	1.73	0.97
1:E:429:ASN:O	1:E:431:ASN:N	1.99	0.96
1:D:429:ASN:CA	1:D:430:ARG:HB3	1.94	0.96
1:C:478:ASP:CA	1:C:479:LYS:CB	2.40	0.95
1:A:353:LEU:C	1:A:354:ILE:HG12	1.86	0.95
1:E:431:ASN:CA	1:E:432:ILE:CB	2.34	0.94
1:B:450:LEU:CD1	1:B:451:LEU:N	2.30	0.94
1:E:432:ILE:H	1:E:493:ARG:CB	1.80	0.93
1:F:4:ALA:HA	1:F:5:ARG:CB	1.96	0.93
1:C:444:GLY:HA3	1:C:445:MET:CB	1.98	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:398:LEU:HD12	1:F:406:ASP:CA	1.99	0.92
1:A:478:ASP:CB	1:A:479:LYS:CB	2.46	0.92
1:B:431:ASN:C	1:B:432:ILE:HG22	1.89	0.92
1:B:449:ARG:N	1:B:482:PHE:CE2	2.38	0.91
1:C:418:GLU:HG3	1:C:419:GLU:HB3	0.95	0.91
1:A:478:ASP:CA	1:A:479:LYS:CB	2.48	0.90
1:F:478:ASP:HB3	1:F:479:LYS:CA	2.02	0.89
1:D:305:ASN:O	1:D:309:ASN:HB2	1.71	0.89
1:F:478:ASP:CB	1:F:479:LYS:HA	2.02	0.89
1:A:431:ASN:HA	1:A:432:ILE:CB	2.03	0.88
1:B:449:ARG:N	1:B:482:PHE:HE2	1.72	0.88
1:B:449:ARG:HG2	1:B:449:ARG:NH1	1.83	0.88
1:D:7:THR:C	1:D:8:VAL:CG2	2.43	0.87
1:A:478:ASP:HA	1:A:479:LYS:CB	2.05	0.87
1:D:429:ASN:HA	1:D:430:ARG:HB2	1.55	0.87
1:B:432:ILE:HG12	1:B:432:ILE:O	1.75	0.87
1:F:445:MET:HA	1:F:446:LYS:CB	2.03	0.86
1:A:478:ASP:CA	1:A:479:LYS:HB2	2.05	0.86
1:B:469:GLY:CA	1:B:470:GLU:CB	2.53	0.85
1:F:432:ILE:O	1:F:433:HIS:CD2	2.30	0.85
1:D:309:ASN:HB3	1:D:310:GLU:HB2	1.57	0.85
1:A:310:GLU:H	1:A:311:PRO:HD3	1.41	0.85
1:E:431:ASN:HA	1:E:432:ILE:HB	0.86	0.84
1:B:480:SER:HA	1:B:481:SER:CB	2.07	0.84
1:F:398:LEU:CD1	1:F:406:ASP:HB3	2.07	0.84
1:F:398:LEU:HD12	1:F:406:ASP:CB	2.08	0.84
1:A:305:ASN:O	1:A:309:ASN:HB2	1.78	0.83
1:F:398:LEU:HD12	1:F:406:ASP:HA	1.57	0.83
1:F:445:MET:HB3	1:F:446:LYS:CB	2.08	0.83
1:B:431:ASN:C	1:B:432:ILE:CG2	2.46	0.83
1:D:7:THR:C	1:D:8:VAL:HG23	1.98	0.82
1:B:368:ALA:O	1:B:369:ALA:HB3	1.77	0.82
1:E:431:ASN:CA	1:E:432:ILE:CG2	2.57	0.82
1:B:353:LEU:HB3	1:B:354:ILE:HG13	1.61	0.82
1:A:431:ASN:OD1	1:A:433:HIS:HB2	1.78	0.82
1:F:445:MET:CB	1:F:446:LYS:CB	2.58	0.81
1:A:432:ILE:O	1:A:432:ILE:HD13	1.81	0.80
1:B:431:ASN:O	1:B:432:ILE:CG2	2.30	0.80
1:B:7:THR:CG2	1:B:393:VAL:HB	2.11	0.80
1:D:309:ASN:ND2	1:D:310:GLU:HG3	1.96	0.80
1:B:353:LEU:C	1:B:354:ILE:HG12	2.01	0.80
1:E:431:ASN:HA	1:E:432:ILE:CG2	2.11	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:432:ILE:CG1	1:B:432:ILE:O	2.30	0.80
1:C:7:THR:CG2	1:C:393:VAL:HB	2.12	0.79
1:B:368:ALA:O	1:B:369:ALA:CB	2.30	0.79
1:B:306:ILE:O	1:B:306:ILE:CG2	2.30	0.79
1:F:445:MET:CA	1:F:446:LYS:CB	2.50	0.79
1:B:431:ASN:O	1:B:432:ILE:HG23	1.83	0.79
1:E:432:ILE:N	1:E:493:ARG:HB2	1.93	0.78
1:E:431:ASN:O	1:E:494:ALA:N	2.13	0.78
1:A:393:VAL:HG21	1:D:12:TYR:CE1	2.19	0.78
1:E:397:PRO:C	1:E:398:LEU:HD23	2.04	0.78
1:D:7:THR:CA	1:D:8:VAL:HG23	2.13	0.78
1:D:7:THR:HA	1:D:8:VAL:HG23	1.66	0.77
1:C:417:ASN:HA	1:C:418:GLU:HB3	1.65	0.77
1:F:431:ASN:HD21	1:F:434:GLU:CG	1.98	0.77
1:A:7:THR:CG2	1:A:393:VAL:HG12	2.14	0.77
1:C:417:ASN:HA	1:C:418:GLU:CB	2.15	0.76
1:D:431:ASN:CA	1:D:432:ILE:HG22	2.16	0.76
1:A:431:ASN:CB	1:A:432:ILE:HG22	2.15	0.76
1:B:469:GLY:CA	1:B:470:GLU:HB2	2.10	0.76
1:F:398:LEU:HD13	1:F:406:ASP:C	2.06	0.76
1:F:398:LEU:CD1	1:F:406:ASP:CA	2.64	0.75
1:E:486:ILE:CG2	1:E:487:LEU:N	2.49	0.75
1:F:7:THR:CG2	1:F:393:VAL:HB	2.16	0.75
1:B:449:ARG:CG	1:B:449:ARG:NH1	2.40	0.75
1:A:7:THR:HG22	1:A:393:VAL:HG12	1.66	0.75
1:F:398:LEU:HD12	1:F:406:ASP:HB3	1.66	0.74
1:E:353:LEU:HB3	1:E:354:ILE:HG12	1.69	0.74
1:D:353:LEU:C	1:D:354:ILE:HG12	2.08	0.74
1:B:429:ASN:O	1:B:494:ALA:HA	1.88	0.74
1:D:310:GLU:H	1:D:311:PRO:HD3	1.50	0.74
1:F:363:GLU:O	1:F:364:ARG:HB2	1.87	0.74
1:A:431:ASN:OD1	1:A:434:GLU:HB2	1.88	0.74
1:B:306:ILE:HG22	1:B:306:ILE:O	1.86	0.74
1:F:353:LEU:HB3	1:F:354:ILE:HG12	1.70	0.74
1:C:363:GLU:O	1:C:364:ARG:HB2	1.87	0.73
1:A:444:GLY:N	1:A:445:MET:HB2	2.03	0.73
1:B:480:SER:HA	1:B:481:SER:HB2	1.69	0.73
1:A:12:TYR:CE2	1:D:12:TYR:CE2	2.77	0.73
1:F:435:ASP:OD1	1:F:493:ARG:HG2	1.89	0.73
1:B:433:HIS:H	1:B:493:ARG:HB2	1.54	0.73
1:A:336:ILE:HG23	1:A:413:VAL:HG22	1.71	0.73
1:F:336:ILE:HG23	1:F:413:VAL:HG22	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:4:ALA:O	1:F:438:LEU:HA	1.89	0.72
1:E:243:GLN:NE2	5:E:2011:HOH:O	2.21	0.72
1:E:336:ILE:HG23	1:E:413:VAL:HG22	1.71	0.72
1:C:469:GLY:HA2	1:C:470:GLU:HB3	1.72	0.72
1:F:469:GLY:HA2	1:F:470:GLU:CB	2.20	0.71
1:F:431:ASN:HA	1:F:432:ILE:HG22	1.72	0.71
1:A:353:LEU:O	1:A:354:ILE:HG12	1.91	0.71
1:F:469:GLY:HA2	1:F:470:GLU:HB3	1.71	0.71
1:E:469:GLY:HA2	1:E:470:GLU:CB	2.20	0.71
1:D:336:ILE:HG23	1:D:413:VAL:HG22	1.71	0.71
1:C:469:GLY:HA2	1:C:470:GLU:CB	2.20	0.71
1:B:336:ILE:HG23	1:B:413:VAL:HG22	1.71	0.71
1:D:409:ASP:O	1:D:429:ASN:CB	2.37	0.70
1:D:309:ASN:C	1:D:310:GLU:CG	2.60	0.70
1:C:478:ASP:HA	1:C:479:LYS:CB	2.13	0.70
1:F:431:ASN:C	1:F:432:ILE:HG22	2.12	0.70
1:E:469:GLY:HA2	1:E:470:GLU:HB3	1.72	0.70
1:D:469:GLY:HA2	1:D:470:GLU:CB	2.20	0.70
1:B:12:TYR:CE2	1:C:12:TYR:CE2	2.80	0.70
1:D:469:GLY:HA2	1:D:470:GLU:HB3	1.73	0.69
1:E:450:LEU:HD22	1:E:481:SER:HA	1.74	0.69
1:D:100:ILE:HG12	1:D:312:TRP:O	1.92	0.69
1:B:431:ASN:OD1	1:B:434:GLU:N	2.22	0.69
1:F:431:ASN:ND2	1:F:434:GLU:CG	2.55	0.69
1:A:310:GLU:N	1:A:311:PRO:HD3	2.08	0.69
1:E:486:ILE:HG22	1:E:487:LEU:N	2.07	0.69
1:C:431:ASN:HD21	1:C:434:GLU:HG3	1.58	0.69
1:C:353:LEU:C	1:C:354:ILE:HG12	2.13	0.69
1:F:477:SER:CA	1:F:478:ASP:OD1	2.41	0.69
1:C:485:GLY:CA	1:C:486:ILE:O	2.38	0.69
1:F:477:SER:C	1:F:478:ASP:OD1	2.31	0.68
1:F:398:LEU:CD1	1:F:406:ASP:C	2.61	0.68
1:F:431:ASN:ND2	1:F:434:GLU:HG3	2.08	0.68
1:D:479:LYS:O	1:D:480:SER:HB2	1.94	0.68
1:B:106:GLY:C	1:B:107:ILE:CG2	2.62	0.67
1:A:431:ASN:HA	1:A:432:ILE:HG22	0.70	0.67
1:D:311:PRO:HB2	1:D:312:TRP:CD1	2.28	0.67
1:C:417:ASN:HA	1:C:418:GLU:HG2	1.76	0.67
1:F:361:VAL:O	1:F:369:ALA:HA	1.94	0.67
1:D:309:ASN:CG	1:D:310:GLU:HG3	2.16	0.67
1:C:100:ILE:HG12	1:C:312:TRP:O	1.95	0.67
1:C:419:GLU:HG3	1:C:420:LYS:HB2	1.75	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:309:ASN:O	1:D:310:GLU:CG	2.43	0.66
1:D:361:VAL:O	1:D:369:ALA:HA	1.94	0.66
1:C:444:GLY:CA	1:C:445:MET:CB	2.73	0.66
1:F:431:ASN:O	1:F:433:HIS:N	2.28	0.66
1:A:393:VAL:HG21	1:D:12:TYR:CZ	2.31	0.66
1:C:361:VAL:O	1:C:369:ALA:HA	1.95	0.66
1:C:417:ASN:OD1	1:C:418:GLU:N	2.30	0.65
1:F:398:LEU:HD11	1:F:406:ASP:HB3	1.78	0.65
1:A:442:VAL:CG2	1:A:445:MET:HB3	2.22	0.65
1:C:429:ASN:O	1:C:429:ASN:CG	2.33	0.65
1:A:42:ASN:ND2	1:A:366:GLY:O	2.22	0.65
1:E:361:VAL:O	1:E:369:ALA:HA	1.95	0.65
1:B:361:VAL:O	1:B:369:ALA:HA	1.96	0.65
1:F:5:ARG:CB	1:F:395:ASN:O	2.45	0.65
1:C:431:ASN:ND2	1:C:431:ASN:O	2.30	0.65
1:F:445:MET:HB3	1:F:446:LYS:HB3	1.79	0.65
1:A:444:GLY:H	1:A:445:MET:HB2	1.62	0.65
1:D:363:GLU:O	1:D:364:ARG:HB2	1.97	0.65
1:D:353:LEU:O	1:D:354:ILE:HG12	1.96	0.65
1:E:410:ILE:HD11	1:E:491:LEU:HD12	1.79	0.65
1:D:380:HIS:HD2	1:D:496:TRP:HE1	1.45	0.65
1:F:365:ASN:N	1:F:365:ASN:OD1	2.30	0.64
1:E:431:ASN:HB2	1:E:433:HIS:H	1.63	0.64
1:A:444:GLY:HA3	1:A:445:MET:CB	2.21	0.64
1:D:7:THR:OG1	1:D:8:VAL:N	2.30	0.64
1:C:429:ASN:C	1:C:431:ASN:H	2.00	0.64
1:C:451:LEU:HD12	1:C:501:ILE:C	2.17	0.64
1:F:410:ILE:HD11	1:F:491:LEU:HD12	1.80	0.64
1:D:410:ILE:HD11	1:D:491:LEU:HD12	1.80	0.64
1:B:380:HIS:HD2	1:B:496:TRP:HE1	1.45	0.64
1:E:380:HIS:HD2	1:E:496:TRP:HE1	1.46	0.64
1:E:431:ASN:O	1:E:493:ARG:HA	1.97	0.63
1:C:410:ILE:HD11	1:C:491:LEU:HD12	1.79	0.63
1:C:417:ASN:O	1:C:422:GLU:N	2.26	0.63
1:C:417:ASN:CG	1:C:418:GLU:HG2	2.18	0.63
1:E:439:VAL:HG12	1:E:488:THR:HG22	1.80	0.63
1:B:429:ASN:OD1	1:B:431:ASN:N	2.32	0.63
1:A:410:ILE:HD11	1:A:491:LEU:HD12	1.80	0.63
1:A:429:ASN:O	1:A:494:ALA:HA	1.97	0.63
1:C:478:ASP:HB3	1:C:479:LYS:CA	2.25	0.63
1:E:429:ASN:O	1:E:431:ASN:C	2.36	0.63
1:A:380:HIS:HD2	1:A:496:TRP:HE1	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:380:HIS:HD2	1:C:496:TRP:HE1	1.46	0.63
1:E:305:ASN:O	1:E:309:ASN:HB2	1.98	0.63
1:A:431:ASN:C	1:A:432:ILE:HG22	2.19	0.62
1:B:410:ILE:HD11	1:B:491:LEU:HD12	1.80	0.62
1:D:100:ILE:CG1	1:D:312:TRP:O	2.46	0.62
1:D:410:ILE:HD12	1:D:429:ASN:HB3	1.81	0.62
1:A:469:GLY:HA2	1:A:470:GLU:HB2	1.81	0.62
1:B:106:GLY:C	1:B:107:ILE:HG23	2.19	0.62
1:B:7:THR:HG22	1:B:393:VAL:HB	1.79	0.62
1:D:309:ASN:ND2	1:D:310:GLU:OE2	2.32	0.62
1:A:453:HIS:ND1	1:A:499:ILE:HG12	2.14	0.62
1:D:453:HIS:ND1	1:D:499:ILE:HG12	2.15	0.62
1:C:453:HIS:ND1	1:C:499:ILE:HG12	2.14	0.62
1:C:408:THR:O	1:C:430:ARG:HD3	2.00	0.62
1:B:353:LEU:O	1:B:354:ILE:HG12	1.99	0.62
1:D:380:HIS:CD2	1:D:496:TRP:HE1	2.18	0.62
1:B:380:HIS:CD2	1:B:496:TRP:HE1	2.18	0.62
1:E:380:HIS:CD2	1:E:496:TRP:HE1	2.18	0.62
1:A:432:ILE:H	1:A:494:ALA:N	1.98	0.62
1:E:429:ASN:C	1:E:431:ASN:N	2.50	0.62
1:D:309:ASN:CB	1:D:310:GLU:HG3	2.29	0.62
1:D:353:LEU:HB3	1:D:354:ILE:HG13	1.80	0.62
1:B:410:ILE:HD12	1:B:429:ASN:HB2	1.81	0.62
1:B:453:HIS:ND1	1:B:499:ILE:HG12	2.15	0.62
1:E:453:HIS:ND1	1:E:499:ILE:HG12	2.15	0.61
1:C:478:ASP:CG	1:C:479:LYS:HB2	2.17	0.61
1:A:380:HIS:CD2	1:A:496:TRP:HE1	2.18	0.61
1:E:429:ASN:O	1:E:429:ASN:CG	2.39	0.61
1:F:453:HIS:ND1	1:F:499:ILE:HG12	2.16	0.61
1:C:7:THR:HG22	1:C:393:VAL:HB	1.81	0.61
1:A:478:ASP:HB3	1:A:479:LYS:CA	2.31	0.61
1:A:442:VAL:HG22	1:A:445:MET:CB	2.26	0.61
1:A:449:ARG:HG2	1:A:449:ARG:O	1.98	0.61
1:E:431:ASN:HB2	1:E:432:ILE:CG2	2.15	0.61
1:F:398:LEU:CD1	1:F:406:ASP:CB	2.72	0.61
1:B:480:SER:HA	1:B:481:SER:HB3	1.82	0.61
1:F:431:ASN:CG	1:F:431:ASN:O	2.38	0.61
1:C:431:ASN:HA	1:C:432:ILE:HB	1.83	0.61
1:C:380:HIS:CD2	1:C:496:TRP:HE1	2.18	0.60
1:C:419:GLU:HG3	1:C:419:GLU:O	2.01	0.60
1:B:408:THR:O	1:B:430:ARG:HD2	2.01	0.60
1:C:479:LYS:O	1:C:480:SER:CB	2.49	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:417:ASN:HA	1:C:418:GLU:CG	2.31	0.60
1:B:480:SER:CA	1:B:481:SER:HB2	2.31	0.59
1:C:100:ILE:CG1	1:C:312:TRP:O	2.50	0.59
1:E:365:ASN:N	1:E:365:ASN:OD1	2.35	0.59
1:C:479:LYS:O	1:C:480:SER:HB3	2.03	0.59
1:F:429:ASN:O	1:F:494:ALA:N	2.35	0.59
1:F:432:ILE:O	1:F:433:HIS:HD2	1.85	0.59
1:B:51:ARG:HH22	1:B:367:GLY:HA3	1.68	0.59
1:D:309:ASN:O	1:D:310:GLU:HG3	2.03	0.59
1:A:353:LEU:HB3	1:A:354:ILE:HG13	1.83	0.59
1:A:368:ALA:O	1:A:369:ALA:HB3	2.01	0.59
1:E:8:VAL:HG22	1:E:442:VAL:HG23	1.85	0.59
1:F:431:ASN:CA	1:F:432:ILE:HG22	2.32	0.58
1:A:310:GLU:H	1:A:311:PRO:CD	2.16	0.58
1:B:353:LEU:HB3	1:B:354:ILE:CG1	2.32	0.58
1:E:431:ASN:C	1:E:494:ALA:N	2.57	0.58
1:D:309:ASN:HB3	1:D:310:GLU:CB	2.31	0.58
1:E:362:THR:HG22	1:E:369:ALA:HB2	1.84	0.58
1:A:410:ILE:HD12	1:A:429:ASN:HB2	1.86	0.58
1:F:353:LEU:CB	1:F:354:ILE:HG12	2.34	0.58
1:C:362:THR:HG22	1:C:369:ALA:HB2	1.85	0.58
1:F:410:ILE:HD12	1:F:429:ASN:HB2	1.86	0.58
1:E:432:ILE:N	1:E:493:ARG:C	2.57	0.58
1:B:469:GLY:HA2	1:B:470:GLU:HB3	1.80	0.58
1:A:469:GLY:HA2	1:A:470:GLU:CB	2.34	0.58
1:D:445:MET:HB2	1:D:447:ASP:H	1.68	0.58
1:D:429:ASN:CB	1:D:430:ARG:HB3	2.34	0.58
1:E:398:LEU:HD23	1:E:398:LEU:N	2.16	0.58
1:A:434:GLU:H	1:A:493:ARG:HB3	1.68	0.57
1:E:431:ASN:C	1:E:494:ALA:H	2.07	0.57
1:F:455:VAL:HG23	1:F:497:ASN:OD1	2.03	0.57
1:F:362:THR:HG22	1:F:369:ALA:HB2	1.85	0.57
1:F:453:HIS:CE1	1:F:497:ASN:ND2	2.72	0.57
1:E:353:LEU:CB	1:E:354:ILE:HG12	2.33	0.57
1:D:362:THR:HG22	1:D:369:ALA:HB2	1.85	0.57
1:E:432:ILE:H	1:E:493:ARG:CA	2.17	0.57
1:A:442:VAL:HG13	1:A:445:MET:C	2.25	0.57
1:C:431:ASN:HA	1:C:432:ILE:HG22	1.85	0.57
1:C:417:ASN:O	1:C:422:GLU:O	2.23	0.57
1:C:417:ASN:OD1	1:C:420:LYS:HB3	2.04	0.57
1:C:417:ASN:OD1	1:C:418:GLU:CG	2.53	0.56
1:D:309:ASN:C	1:D:310:GLU:HG3	2.24	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:458:HIS:HD2	1:F:460:ASP:H	1.53	0.56
1:B:481:SER:HB3	1:B:488:THR:O	2.06	0.56
1:B:51:ARG:HH12	1:B:367:GLY:CA	2.18	0.56
1:C:491:LEU:HD22	1:C:497:ASN:ND2	2.21	0.56
1:A:431:ASN:CA	1:A:432:ILE:CB	2.78	0.56
1:A:478:ASP:CG	1:A:479:LYS:HB3	2.25	0.56
1:F:380:HIS:CD2	1:F:496:TRP:HE1	2.24	0.56
1:C:419:GLU:O	1:C:419:GLU:CG	2.53	0.56
1:C:339:MET:HE1	1:C:413:VAL:CG1	2.36	0.56
1:B:100:ILE:HG12	1:B:312:TRP:O	2.05	0.56
1:B:477:SER:HB2	1:B:478:ASP:OD1	2.06	0.56
1:E:458:HIS:HD2	1:E:460:ASP:H	1.54	0.56
1:B:469:GLY:CA	1:B:470:GLU:HB3	2.35	0.56
1:C:431:ASN:HA	1:C:432:ILE:CB	2.36	0.56
1:B:429:ASN:O	1:B:494:ALA:CA	2.54	0.55
1:B:458:HIS:HD2	1:B:460:ASP:H	1.54	0.55
1:B:480:SER:CA	1:B:481:SER:CB	2.81	0.55
1:E:431:ASN:HB2	1:E:433:HIS:N	2.21	0.55
1:D:458:HIS:HD2	1:D:460:ASP:H	1.54	0.55
1:B:491:LEU:HD22	1:B:497:ASN:ND2	2.21	0.55
1:B:354:ILE:H	1:B:358:ALA:CB	2.20	0.55
1:D:257:ALA:HA	1:D:430:ARG:NH1	2.21	0.55
1:A:458:HIS:HD2	1:A:460:ASP:H	1.54	0.55
1:F:398:LEU:CD1	1:F:406:ASP:HA	2.32	0.55
1:D:305:ASN:O	1:D:309:ASN:CB	2.48	0.55
1:B:353:LEU:C	1:B:354:ILE:CG1	2.73	0.55
1:D:310:GLU:N	1:D:311:PRO:HD3	2.22	0.55
1:E:491:LEU:HD22	1:E:497:ASN:ND2	2.21	0.55
1:F:449:ARG:O	1:F:449:ARG:HG2	2.05	0.55
1:D:491:LEU:HD22	1:D:497:ASN:ND2	2.22	0.54
1:E:8:VAL:HG22	1:E:8:VAL:O	2.06	0.54
1:B:431:ASN:OD1	1:B:434:GLU:HB2	2.07	0.54
1:D:309:ASN:O	1:D:310:GLU:HG2	2.06	0.54
1:B:393:VAL:HG22	1:C:12:TYR:OH	2.08	0.54
1:A:491:LEU:HD22	1:A:497:ASN:ND2	2.22	0.54
1:A:429:ASN:C	1:A:431:ASN:H	2.11	0.54
1:A:432:ILE:H	1:A:493:ARG:C	2.11	0.54
1:D:42:ASN:ND2	1:D:366:GLY:O	2.41	0.54
1:D:445:MET:HG3	1:D:448:TYR:CG	2.42	0.54
1:A:393:VAL:CG2	1:D:12:TYR:CE1	2.90	0.54
1:B:100:ILE:CG1	1:B:312:TRP:O	2.56	0.53
1:B:12:TYR:OH	1:C:393:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:7:THR:HG23	1:F:393:VAL:HB	1.91	0.53
1:C:431:ASN:HA	1:C:432:ILE:CG2	2.38	0.53
1:C:398:LEU:N	1:C:398:LEU:HD23	2.22	0.53
1:D:7:THR:C	1:D:8:VAL:HG22	2.27	0.53
1:E:311:PRO:HB2	1:E:312:TRP:CD1	2.44	0.53
1:F:311:PRO:HB2	1:F:312:TRP:CD1	2.43	0.53
1:C:417:ASN:CA	1:C:418:GLU:HG2	2.38	0.53
1:D:354:ILE:H	1:D:358:ALA:CB	2.22	0.53
1:E:397:PRO:O	1:E:398:LEU:HD23	2.09	0.53
1:D:309:ASN:ND2	1:D:310:GLU:CG	2.69	0.52
1:B:432:ILE:O	1:B:433:HIS:CD2	2.63	0.52
1:C:397:PRO:C	1:C:398:LEU:HD23	2.30	0.52
1:F:51:ARG:HH12	1:F:367:GLY:HA3	1.74	0.52
1:E:468:ASN:O	1:E:469:GLY:O	2.27	0.52
1:C:42:ASN:ND2	1:C:366:GLY:O	2.39	0.52
1:E:435:ASP:OD1	1:E:493:ARG:HG2	2.10	0.52
1:C:477:SER:HB2	1:C:478:ASP:OD1	2.09	0.52
1:A:433:HIS:N	1:A:493:ARG:HB2	2.25	0.52
1:C:449:ARG:HA	1:C:482:PHE:CD2	2.45	0.52
1:D:429:ASN:O	1:D:429:ASN:CG	2.48	0.51
1:B:431:ASN:O	1:B:433:HIS:HB2	2.10	0.51
1:F:491:LEU:HD22	1:F:497:ASN:ND2	2.24	0.51
1:F:7:THR:HG22	1:F:393:VAL:HB	1.91	0.51
1:D:431:ASN:O	1:D:431:ASN:CG	2.48	0.51
1:A:477:SER:HB2	1:A:478:ASP:OD1	2.10	0.51
1:D:364:ARG:O	1:D:365:ASN:C	2.49	0.51
1:B:364:ARG:O	1:B:365:ASN:C	2.49	0.51
1:C:354:ILE:H	1:C:358:ALA:CB	2.23	0.51
1:A:432:ILE:H	1:A:493:ARG:CA	2.24	0.51
1:D:67:ARG:HD2	1:D:291:ASP:HB2	1.93	0.51
1:F:398:LEU:CD1	1:F:406:ASP:O	2.59	0.51
1:D:353:LEU:C	1:D:354:ILE:CG1	2.75	0.51
1:D:429:ASN:HB2	1:D:430:ARG:HB3	1.93	0.50
1:C:451:LEU:CD1	1:C:501:ILE:C	2.80	0.50
1:C:175:ASP:OD1	1:C:214:SER:OG	2.28	0.50
1:B:175:ASP:OD1	1:B:214:SER:OG	2.29	0.50
1:E:8:VAL:CG2	1:E:8:VAL:O	2.59	0.50
1:A:188:TYR:HA	1:A:191:ILE:HG22	1.93	0.50
1:B:67:ARG:HD2	1:B:291:ASP:HB2	1.93	0.50
1:C:417:ASN:OD1	1:C:418:GLU:HG2	2.11	0.50
1:B:188:TYR:HA	1:B:191:ILE:HG22	1.93	0.50
1:B:429:ASN:O	1:B:494:ALA:N	2.43	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:478:ASP:HB3	1:B:479:LYS:CB	2.42	0.50
1:A:393:VAL:CG2	1:D:12:TYR:CZ	2.94	0.50
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.93	0.50
1:E:67:ARG:HD2	1:E:291:ASP:HB2	1.93	0.50
1:F:4:ALA:CB	1:F:395:ASN:O	2.60	0.50
1:B:480:SER:HB2	1:B:489:SER:HA	1.93	0.50
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.93	0.50
1:E:429:ASN:O	1:E:429:ASN:OD1	2.30	0.50
1:E:429:ASN:O	1:E:431:ASN:CA	2.60	0.50
1:C:307:MET:O	1:C:308:GLN:HB2	2.12	0.50
1:F:432:ILE:HD13	1:F:433:HIS:CD2	2.47	0.50
1:F:431:ASN:OD1	1:F:431:ASN:O	2.30	0.50
1:C:429:ASN:C	1:C:431:ASN:N	2.65	0.50
1:F:67:ARG:HD2	1:F:291:ASP:HB2	1.94	0.50
1:C:429:ASN:O	1:C:429:ASN:OD1	2.30	0.49
1:E:8:VAL:CG2	1:E:442:VAL:HG23	2.42	0.49
1:D:445:MET:SD	1:D:445:MET:N	2.85	0.49
1:F:398:LEU:HD13	1:F:406:ASP:O	2.10	0.49
1:B:51:ARG:HH12	1:B:367:GLY:HA2	1.76	0.49
1:A:361:VAL:O	1:A:369:ALA:HA	2.12	0.49
1:A:451:LEU:HB2	1:A:500:ARG:O	2.12	0.49
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.93	0.49
1:F:431:ASN:HD21	1:F:434:GLU:HG3	1.73	0.49
1:E:449:ARG:HG2	1:E:449:ARG:O	2.12	0.49
1:D:175:ASP:OD1	1:D:214:SER:OG	2.28	0.49
1:E:478:ASP:HB3	1:E:479:LYS:CB	2.43	0.49
1:B:432:ILE:CD1	1:B:432:ILE:O	2.59	0.49
1:C:458:HIS:HD2	1:C:460:ASP:H	1.61	0.49
1:F:453:HIS:CE1	1:F:497:ASN:HD22	2.31	0.49
1:C:339:MET:CE	1:C:413:VAL:CG1	2.90	0.49
1:A:10:LYS:HD2	1:A:11:ASP:OD1	2.12	0.49
1:A:67:ARG:HD2	1:A:291:ASP:HB2	1.93	0.49
1:C:480:SER:HB2	1:C:489:SER:HA	1.95	0.49
1:A:353:LEU:HB3	1:A:354:ILE:CG1	2.41	0.49
1:B:354:ILE:H	1:B:358:ALA:HB2	1.77	0.49
1:C:67:ARG:HD2	1:C:291:ASP:HB2	1.93	0.49
1:C:7:THR:HG23	1:C:393:VAL:HB	1.93	0.49
1:A:363:GLU:O	1:A:364:ARG:HB2	2.13	0.49
1:A:442:VAL:HG11	1:A:482:PHE:HZ	1.78	0.49
1:D:431:ASN:O	1:D:431:ASN:OD1	2.30	0.49
1:B:479:LYS:O	1:B:480:SER:HB3	2.12	0.49
1:C:431:ASN:CG	1:C:431:ASN:O	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:175:ASP:OD1	1:F:214:SER:OG	2.27	0.49
1:F:42:ASN:ND2	1:F:366:GLY:O	2.29	0.49
1:B:450:LEU:CD1	1:B:451:LEU:H	2.22	0.48
1:E:188:TYR:HA	1:E:191:ILE:HG22	1.93	0.48
1:F:4:ALA:HB1	1:F:395:ASN:O	2.13	0.48
1:A:310:GLU:N	1:A:311:PRO:CD	2.76	0.48
1:B:353:LEU:CB	1:B:354:ILE:HG13	2.38	0.48
1:A:175:ASP:OD1	1:A:214:SER:OG	2.28	0.48
1:F:429:ASN:OD1	1:F:431:ASN:HB3	2.13	0.48
1:E:480:SER:HB2	1:E:489:SER:HA	1.95	0.48
1:A:293:TRP:O	1:A:294:ASN:HB2	2.14	0.48
1:B:293:TRP:O	1:B:294:ASN:HB2	2.13	0.48
1:A:431:ASN:O	1:A:431:ASN:OD1	2.30	0.48
1:E:456:LEU:HB3	1:E:496:TRP:HB3	1.95	0.48
1:A:444:GLY:HA3	1:A:445:MET:SD	2.53	0.48
1:D:366:GLY:HA3	1:D:367:GLY:HA2	1.49	0.48
1:E:42:ASN:ND2	1:E:366:GLY:O	2.45	0.48
1:C:354:ILE:H	1:C:358:ALA:HB2	1.79	0.48
1:A:456:LEU:HB3	1:A:496:TRP:HB3	1.96	0.48
1:E:486:ILE:HG23	1:E:487:LEU:H	1.78	0.48
1:B:456:LEU:HB3	1:B:496:TRP:HB3	1.95	0.47
1:E:175:ASP:OD1	1:E:214:SER:OG	2.29	0.47
1:E:424:THR:HG23	1:E:500:ARG:HG2	1.96	0.47
1:B:435:ASP:OD1	1:B:493:ARG:HG2	2.14	0.47
1:B:354:ILE:N	1:B:358:ALA:HB1	2.29	0.47
1:F:435:ASP:OD1	1:F:493:ARG:CG	2.62	0.47
1:D:456:LEU:HB3	1:D:496:TRP:HB3	1.95	0.47
1:A:368:ALA:O	1:A:369:ALA:CB	2.62	0.47
1:C:456:LEU:HB3	1:C:496:TRP:HB3	1.95	0.47
1:C:417:ASN:OD1	1:C:418:GLU:HG3	2.14	0.47
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.57	0.47
1:E:432:ILE:N	1:E:493:ARG:CA	2.77	0.47
1:F:453:HIS:HE1	1:F:497:ASN:HD22	1.63	0.47
1:B:424:THR:HG23	1:B:500:ARG:HG2	1.97	0.47
1:F:456:LEU:HB3	1:F:496:TRP:HB3	1.97	0.47
1:C:424:THR:HG23	1:C:500:ARG:HG2	1.96	0.47
1:D:354:ILE:H	1:D:358:ALA:HB2	1.79	0.47
1:F:424:THR:HG23	1:F:500:ARG:HG2	1.97	0.47
1:B:479:LYS:O	1:B:480:SER:CB	2.62	0.47
1:B:12:TYR:HE2	1:C:12:TYR:CE2	2.32	0.47
1:C:293:TRP:O	1:C:294:ASN:HB2	2.15	0.47
1:E:431:ASN:OD1	1:E:431:ASN:N	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:ASN:O	1:A:309:ASN:CB	2.57	0.47
1:B:51:ARG:NH2	1:B:367:GLY:HA3	2.29	0.47
1:D:256:LEU:O	1:D:430:ARG:NH1	2.48	0.46
1:A:351:ALA:HA	1:A:352:GLN:HA	1.69	0.46
1:F:293:TRP:O	1:F:294:ASN:HB2	2.14	0.46
1:D:293:TRP:O	1:D:294:ASN:HB2	2.15	0.46
1:A:429:ASN:O	1:A:494:ALA:N	2.48	0.46
1:D:309:ASN:HD22	1:D:310:GLU:CG	2.28	0.46
1:D:453:HIS:CE1	1:D:499:ILE:HG12	2.51	0.46
1:A:424:THR:HG23	1:A:500:ARG:HG2	1.97	0.46
1:D:429:ASN:O	1:D:494:ALA:HA	2.16	0.46
1:D:354:ILE:N	1:D:358:ALA:HB1	2.31	0.46
1:F:431:ASN:ND2	1:F:434:GLU:HG2	2.29	0.46
1:A:354:ILE:H	1:A:358:ALA:CB	2.28	0.46
1:C:353:LEU:HB3	1:C:354:ILE:HG13	1.98	0.46
1:C:449:ARG:O	1:C:501:ILE:HG23	2.14	0.46
1:A:453:HIS:CE1	1:A:499:ILE:HG12	2.51	0.46
1:F:351:ALA:HA	1:F:352:GLN:HA	1.68	0.46
1:C:431:ASN:C	1:C:433:HIS:H	2.16	0.46
1:D:306:ILE:HG21	1:D:318:LEU:CD2	2.45	0.46
1:E:203:ASP:O	1:E:206:ILE:HG12	2.16	0.46
1:D:424:THR:HG23	1:D:500:ARG:HG2	1.97	0.46
1:E:479:LYS:O	1:E:480:SER:HB3	2.14	0.46
1:F:481:SER:OG	1:F:481:SER:O	2.34	0.46
1:B:203:ASP:O	1:B:206:ILE:HG12	2.16	0.46
1:E:293:TRP:O	1:E:294:ASN:HB2	2.14	0.46
1:D:429:ASN:CA	1:D:430:ARG:CB	2.52	0.46
1:B:432:ILE:HD13	1:B:432:ILE:O	2.16	0.46
1:D:431:ASN:C	1:D:433:HIS:H	2.16	0.46
1:F:203:ASP:O	1:F:206:ILE:HG12	2.16	0.46
1:C:106:GLY:O	1:C:108:ASN:N	2.49	0.46
1:C:432:ILE:O	1:C:432:ILE:HD13	2.16	0.45
1:B:453:HIS:CE1	1:B:499:ILE:HG12	2.51	0.45
1:C:428:VAL:CG1	1:C:429:ASN:N	2.79	0.45
1:C:354:ILE:N	1:C:358:ALA:HB1	2.31	0.45
1:D:484:ASP:HA	1:D:485:GLY:HA2	1.53	0.45
1:E:479:LYS:O	1:E:480:SER:CB	2.64	0.45
1:A:106:GLY:O	1:A:108:ASN:N	2.49	0.45
1:A:203:ASP:O	1:A:206:ILE:HG12	2.16	0.45
1:D:363:GLU:HB2	1:D:367:GLY:C	2.37	0.45
1:E:453:HIS:CE1	1:E:499:ILE:HG12	2.52	0.45
1:D:447:ASP:CA	1:D:448:TYR:HB2	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:106:GLY:O	1:D:108:ASN:N	2.49	0.45
1:A:431:ASN:C	1:A:431:ASN:OD1	2.53	0.45
1:C:453:HIS:CE1	1:C:499:ILE:HG12	2.51	0.45
1:B:430:ARG:O	1:B:430:ARG:HG3	2.16	0.45
1:B:311:PRO:HB2	1:B:312:TRP:CD1	2.51	0.45
1:B:7:THR:HG23	1:B:393:VAL:HB	1.92	0.45
1:D:203:ASP:O	1:D:206:ILE:HG12	2.17	0.45
1:C:478:ASP:CG	1:C:479:LYS:CB	2.81	0.45
1:D:7:THR:O	1:D:8:VAL:HG22	2.17	0.45
1:F:453:HIS:CE1	1:F:499:ILE:HG12	2.52	0.45
1:A:429:ASN:O	1:A:494:ALA:CA	2.63	0.45
1:B:168:TRP:HB2	1:B:208:LEU:HD23	1.99	0.45
1:D:306:ILE:CG2	1:D:318:LEU:HD21	2.46	0.45
1:C:325:PHE:CZ	1:C:457:GLU:HA	2.52	0.45
1:C:203:ASP:O	1:C:206:ILE:HG12	2.17	0.45
1:B:381:ALA:HA	1:B:426:PHE:CE2	2.52	0.44
1:F:432:ILE:HD13	1:F:432:ILE:O	2.18	0.44
1:E:325:PHE:CZ	1:E:457:GLU:HA	2.53	0.44
1:E:106:GLY:O	1:E:108:ASN:N	2.50	0.44
1:F:106:GLY:O	1:F:108:ASN:N	2.50	0.44
1:A:429:ASN:C	1:A:431:ASN:N	2.70	0.44
1:E:429:ASN:C	1:E:431:ASN:H	2.17	0.44
1:F:487:LEU:HG	1:F:488:THR:CA	2.47	0.44
1:B:351:ALA:HA	1:B:352:GLN:HA	1.68	0.44
1:A:325:PHE:CZ	1:A:457:GLU:HA	2.53	0.44
1:C:444:GLY:HA3	1:C:445:MET:HB3	1.93	0.44
1:E:450:LEU:HD22	1:E:481:SER:CA	2.43	0.44
1:A:168:TRP:HB2	1:A:208:LEU:HD23	2.00	0.44
1:D:309:ASN:HD22	1:D:310:GLU:CD	2.20	0.44
1:B:306:ILE:O	1:B:306:ILE:HG23	2.15	0.44
1:C:168:TRP:HB2	1:C:208:LEU:HD23	2.00	0.44
1:D:365:ASN:OD1	1:D:365:ASN:N	2.51	0.44
1:C:398:LEU:HD13	1:C:406:ASP:HB3	1.98	0.44
1:E:168:TRP:HB2	1:E:208:LEU:HD23	2.00	0.44
1:D:168:TRP:HB2	1:D:208:LEU:HD23	2.00	0.44
1:F:325:PHE:CZ	1:F:457:GLU:HA	2.53	0.44
1:C:478:ASP:HA	1:C:479:LYS:CG	2.48	0.44
1:A:431:ASN:O	1:A:431:ASN:CG	2.55	0.44
1:C:417:ASN:CA	1:C:418:GLU:CB	2.93	0.44
1:B:429:ASN:OD1	1:B:431:ASN:HB3	2.18	0.44
1:C:451:LEU:HD12	1:C:502:GLY:N	2.33	0.44
1:D:381:ALA:HA	1:D:426:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:TYR:CE2	1:C:12:TYR:HE2	2.33	0.43
1:C:339:MET:CE	1:C:413:VAL:HG11	2.48	0.43
1:D:325:PHE:CZ	1:D:457:GLU:HA	2.53	0.43
1:F:481:SER:O	1:F:488:THR:CA	2.66	0.43
1:F:381:ALA:HA	1:F:426:PHE:CE2	2.53	0.43
1:F:168:TRP:HB2	1:F:208:LEU:HD23	2.00	0.43
1:E:486:ILE:CG2	1:E:487:LEU:H	2.29	0.43
1:C:381:ALA:HA	1:C:426:PHE:CE2	2.54	0.43
1:A:381:ALA:HA	1:A:426:PHE:CE2	2.54	0.43
1:D:309:ASN:HB3	1:D:310:GLU:HG3	2.00	0.43
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.52	0.43
1:E:364:ARG:O	1:E:365:ASN:C	2.56	0.43
1:E:478:ASP:HA	1:E:479:LYS:CB	2.49	0.43
1:B:325:PHE:CZ	1:B:457:GLU:HA	2.53	0.43
1:F:4:ALA:O	1:F:439:VAL:N	2.45	0.43
1:B:478:ASP:HA	1:B:479:LYS:CB	2.49	0.43
1:B:450:LEU:CD1	1:B:452:GLU:N	2.81	0.42
1:A:354:ILE:H	1:A:358:ALA:HB2	1.83	0.42
1:B:478:ASP:CA	1:B:479:LYS:CB	2.97	0.42
1:E:478:ASP:CA	1:E:479:LYS:CB	2.97	0.42
1:C:417:ASN:C	1:C:417:ASN:OD1	2.57	0.42
1:A:354:ILE:N	1:A:358:ALA:HB1	2.34	0.42
1:D:100:ILE:HG13	1:D:312:TRP:O	2.18	0.42
1:F:380:HIS:HD2	1:F:496:TRP:NE1	2.17	0.42
1:C:451:LEU:HD12	1:C:501:ILE:CA	2.49	0.42
1:B:353:LEU:CB	1:B:354:ILE:CG1	2.97	0.42
2:D:1504:HRH:H2'	2:D:1505:HRH:H4'	2.00	0.42
1:F:144:HIS:HA	1:F:145:PRO:HD3	1.95	0.42
1:D:435:ASP:OD1	1:D:493:ARG:HG2	2.20	0.42
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.92	0.42
1:F:429:ASN:O	1:F:494:ALA:HA	2.19	0.42
1:E:458:HIS:CD2	1:E:460:ASP:H	2.36	0.42
1:A:458:HIS:CD2	1:A:460:ASP:H	2.36	0.42
1:D:351:ALA:HA	1:D:352:GLN:HA	1.69	0.42
1:E:381:ALA:HA	1:E:426:PHE:CE2	2.54	0.42
1:E:309:ASN:O	1:E:310:GLU:HG2	2.20	0.42
1:C:417:ASN:CB	1:C:418:GLU:HG2	2.50	0.42
1:D:15:ALA:HB2	1:D:343:ASP:HB3	2.02	0.42
1:A:431:ASN:O	1:A:434:GLU:O	2.37	0.41
1:A:482:PHE:HD1	1:A:482:PHE:HA	1.68	0.41
1:D:114:CYS:HA	1:D:117:VAL:HG22	2.01	0.41
1:D:368:ALA:O	1:D:369:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:366:GLY:HA3	1:E:367:GLY:HA2	1.37	0.41
1:F:458:HIS:CD2	1:F:460:ASP:H	2.36	0.41
1:C:241:LEU:C	1:C:242:HIS:HD2	2.23	0.41
1:B:214:SER:O	1:B:242:HIS:HB2	2.20	0.41
1:B:434:GLU:C	1:B:493:ARG:HB3	2.41	0.41
1:D:431:ASN:O	1:D:433:HIS:N	2.38	0.41
1:A:380:HIS:HD2	1:A:496:TRP:NE1	2.16	0.41
1:A:10:LYS:H	1:A:10:LYS:HG3	1.62	0.41
1:A:214:SER:O	1:A:242:HIS:HB2	2.21	0.41
1:E:214:SER:O	1:E:242:HIS:HB2	2.20	0.41
1:F:114:CYS:HA	1:F:117:VAL:HG22	2.01	0.41
1:C:409:ASP:O	1:C:430:ARG:HB3	2.21	0.41
1:C:214:SER:O	1:C:242:HIS:HB2	2.20	0.41
1:F:214:SER:O	1:F:242:HIS:HB2	2.20	0.41
1:E:241:LEU:C	1:E:242:HIS:HD2	2.24	0.41
1:B:15:ALA:HB2	1:B:343:ASP:HB3	2.02	0.41
1:D:214:SER:O	1:D:242:HIS:HB2	2.21	0.41
1:A:114:CYS:HA	1:A:117:VAL:HG22	2.01	0.41
1:A:369:ALA:O	1:A:370:TRP:HB3	2.19	0.41
1:C:15:ALA:HB2	1:C:343:ASP:HB3	2.02	0.41
1:D:10:LYS:HD2	1:D:11:ASP:OD1	2.21	0.41
1:F:306:ILE:O	1:F:306:ILE:HG22	2.21	0.41
1:A:431:ASN:CA	1:A:432:ILE:CG2	2.30	0.41
1:E:432:ILE:N	1:E:493:ARG:CB	2.64	0.41
1:A:7:THR:HG21	1:A:393:VAL:HG12	2.01	0.41
1:C:461:LEU:HD12	1:C:461:LEU:HA	1.88	0.41
1:D:380:HIS:HD2	1:D:496:TRP:NE1	2.15	0.40
1:C:144:HIS:HA	1:C:145:PRO:HD3	1.96	0.40
1:C:368:ALA:O	1:C:369:ALA:HB3	2.21	0.40
1:E:63:VAL:HA	1:E:64:PRO:HD3	1.92	0.40
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.02	0.40
1:E:15:ALA:HB2	1:E:343:ASP:HB3	2.02	0.40
1:B:114:CYS:HA	1:B:117:VAL:HG22	2.02	0.40
1:E:451:LEU:O	1:E:452:GLU:HB3	2.21	0.40
1:D:63:VAL:HA	1:D:64:PRO:HD3	1.92	0.40
1:A:15:ALA:HB2	1:A:343:ASP:HB3	2.02	0.40
1:A:353:LEU:HG	1:A:354:ILE:HG12	2.03	0.40
1:C:311:PRO:HB2	1:C:312:TRP:CD1	2.56	0.40
1:C:451:LEU:CD1	1:C:502:GLY:N	2.84	0.40
1:D:241:LEU:C	1:D:242:HIS:HD2	2.25	0.40
1:C:351:ALA:HA	1:C:352:GLN:HA	1.68	0.40
1:C:114:CYS:HA	1:C:117:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:477:SER:HB2	1:D:478:ASP:OD1	2.21	0.40
1:A:433:HIS:HB3	1:A:434:GLU:HG3	2.02	0.40
1:C:353:LEU:O	1:C:354:ILE:HG12	2.20	0.40
1:E:477:SER:HB2	1:E:478:ASP:OD1	2.22	0.40
1:D:431:ASN:C	1:D:432:ILE:HG22	2.42	0.40
1:F:431:ASN:HD21	1:F:434:GLU:HG2	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/513 (96%)	445 (91%)	26 (5%)	19 (4%)	5	10
1	B	493/513 (96%)	440 (89%)	28 (6%)	25 (5%)	3	5
1	C	493/513 (96%)	438 (89%)	30 (6%)	25 (5%)	3	5
1	D	497/513 (97%)	445 (90%)	31 (6%)	21 (4%)	4	8
1	E	484/513 (94%)	438 (90%)	27 (6%)	19 (4%)	5	10
1	F	490/513 (96%)	442 (90%)	27 (6%)	21 (4%)	4	8
All	All	2947/3078 (96%)	2648 (90%)	169 (6%)	130 (4%)	4	8

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	TRP
1	A	309	ASN
1	A	310	GLU
1	A	354	ILE
1	A	365	ASN
1	A	370	TRP
1	A	430	ARG
1	A	432	ILE
1	A	434	GLU

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Mol	Chain	Res	Type
1	A	478	ASP
1	B	46	ASP
1	B	108	ASN
1	B	224	TRP
1	B	305	ASN
1	B	309	ASN
1	B	313	ARG
1	B	354	ILE
1	B	365	ASN
1	B	430	ARG
1	B	433	HIS
1	B	479	LYS
1	B	480	SER
1	B	481	SER
1	B	490	MET
1	C	224	TRP
1	C	313	ARG
1	C	354	ILE
1	C	419	GLU
1	C	430	ARG
1	C	432	ILE
1	C	451	LEU
1	C	478	ASP
1	C	479	LYS
1	C	480	SER
1	C	481	SER
1	C	486	ILE
1	D	8	VAL
1	D	224	TRP
1	D	310	GLU
1	D	313	ARG
1	D	354	ILE
1	D	365	ASN
1	D	432	ILE
1	D	446	LYS
1	D	478	ASP
1	D	479	LYS
1	D	480	SER
1	E	365	ASN
1	E	430	ARG
1	E	432	ILE
1	E	479	LYS

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Mol	Chain	Res	Type
1	E	480	SER
1	F	5	ARG
1	F	365	ASN
1	F	430	ARG
1	F	478	ASP
1	F	488	THR
1	A	107	ILE
1	A	363	GLU
1	B	107	ILE
1	B	363	GLU
1	B	369	ALA
1	B	478	ASP
1	C	107	ILE
1	C	309	ASN
1	C	364	ARG
1	C	365	ASN
1	C	420	LYS
1	C	470	GLU
1	D	363	GLU
1	D	470	GLU
1	E	309	ASN
1	E	310	GLU
1	E	313	ARG
1	E	469	GLY
1	E	470	GLU
1	E	478	ASP
1	F	309	ASN
1	F	310	GLU
1	F	313	ARG
1	F	364	ARG
1	F	470	GLU
1	A	364	ARG
1	A	484	ASP
1	B	307	MET
1	B	308	GLN
1	B	494	ALA
1	C	363	GLU
1	C	369	ALA
1	C	418	GLU
1	D	107	ILE
1	D	312	TRP
1	D	369	ALA

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Mol	Chain	Res	Type
1	E	107	ILE
1	E	363	GLU
1	E	364	ARG
1	E	369	ALA
1	F	107	ILE
1	F	363	GLU
1	F	369	ALA
1	F	494	ALA
1	A	297	TYR
1	A	366	GLY
1	A	369	ALA
1	A	494	ALA
1	B	364	ARG
1	C	297	TYR
1	C	494	ALA
1	D	364	ARG
1	D	494	ALA
1	E	297	TYR
1	E	494	ALA
1	F	432	ILE
1	F	433	HIS
1	F	485	GLY
1	A	357	ILE
1	B	297	TYR
1	B	357	ILE
1	C	357	ILE
1	D	297	TYR
1	D	357	ILE
1	D	449	ARG
1	E	357	ILE
1	F	297	TYR
1	F	357	ILE
1	B	469	GLY
1	C	310	GLU
1	F	469	GLY
1	E	354	ILE
1	F	354	ILE

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	428/450 (95%)	400 (94%)	28 (6%)	24	51
1	B	427/450 (95%)	397 (93%)	30 (7%)	21	47
1	C	428/450 (95%)	395 (92%)	33 (8%)	18	40
1	D	428/450 (95%)	400 (94%)	28 (6%)	24	51
1	E	415/450 (92%)	392 (94%)	23 (6%)	30	60
1	F	425/450 (94%)	396 (93%)	29 (7%)	22	48
All	All	2551/2700 (94%)	2380 (93%)	171 (7%)	23	49

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	TYR
1	A	13	LYS
1	A	44	LYS
1	A	47	GLU
1	A	73	PHE
1	A	87	GLU
1	A	98	LYS
1	A	107	ILE
1	A	160	LYS
1	A	179	GLN
1	A	290	PHE
1	A	365	ASN
1	A	395	ASN
1	A	410	ILE
1	A	413	VAL
1	A	415	ILE
1	A	418	GLU
1	A	430	ARG
1	A	432	ILE
1	A	445	MET
1	A	463	ILE
1	A	470	GLU
1	A	477	SER
1	A	482	PHE
1	A	483	ASP
1	A	484	ASP

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Mol	Chain	Res	Type
1	A	488	THR
1	B	10	LYS
1	B	12	TYR
1	B	13	LYS
1	B	44	LYS
1	B	46	ASP
1	B	47	GLU
1	B	87	GLU
1	B	98	LYS
1	B	107	ILE
1	B	160	LYS
1	B	179	GLN
1	B	290	PHE
1	B	364	ARG
1	B	365	ASN
1	B	393	VAL
1	B	395	ASN
1	B	410	ILE
1	B	413	VAL
1	B	415	ILE
1	B	430	ARG
1	B	432	ILE
1	B	443	ARG
1	B	445	MET
1	B	449	ARG
1	B	450	LEU
1	B	459	GLN
1	B	463	ILE
1	B	468	ASN
1	B	480	SER
1	B	493	ARG
1	C	12	TYR
1	C	13	LYS
1	C	44	LYS
1	C	47	GLU
1	C	87	GLU
1	C	98	LYS
1	C	107	ILE
1	C	160	LYS
1	C	179	GLN
1	C	290	PHE
1	C	308	GLN

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Mol	Chain	Res	Type
1	C	365	ASN
1	C	393	VAL
1	C	395	ASN
1	C	410	ILE
1	C	413	VAL
1	C	415	ILE
1	C	419	GLU
1	C	432	ILE
1	C	434	GLU
1	C	442	VAL
1	C	449	ARG
1	C	451	LEU
1	C	459	GLN
1	C	461	LEU
1	C	463	ILE
1	C	468	ASN
1	C	470	GLU
1	C	477	SER
1	C	480	SER
1	C	483	ASP
1	C	492	ARG
1	C	493	ARG
1	D	7	THR
1	D	10	LYS
1	D	12	TYR
1	D	13	LYS
1	D	44	LYS
1	D	47	GLU
1	D	87	GLU
1	D	98	LYS
1	D	107	ILE
1	D	160	LYS
1	D	179	GLN
1	D	290	PHE
1	D	306	ILE
1	D	354	ILE
1	D	365	ASN
1	D	395	ASN
1	D	410	ILE
1	D	413	VAL
1	D	415	ILE
1	D	429	ASN

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Mol	Chain	Res	Type
1	D	430	ARG
1	D	432	ILE
1	D	445	MET
1	D	459	GLN
1	D	463	ILE
1	D	468	ASN
1	D	470	GLU
1	D	480	SER
1	E	8	VAL
1	E	12	TYR
1	E	13	LYS
1	E	44	LYS
1	E	47	GLU
1	E	87	GLU
1	E	98	LYS
1	E	107	ILE
1	E	160	LYS
1	E	179	GLN
1	E	290	PHE
1	E	365	ASN
1	E	395	ASN
1	E	410	ILE
1	E	413	VAL
1	E	415	ILE
1	E	432	ILE
1	E	451	LEU
1	E	463	ILE
1	E	468	ASN
1	E	470	GLU
1	E	480	SER
1	E	486	ILE
1	F	12	TYR
1	F	13	LYS
1	F	44	LYS
1	F	47	GLU
1	F	87	GLU
1	F	98	LYS
1	F	107	ILE
1	F	160	LYS
1	F	179	GLN
1	F	290	PHE
1	F	310	GLU

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Mol	Chain	Res	Type
1	F	365	ASN
1	F	395	ASN
1	F	398	LEU
1	F	410	ILE
1	F	413	VAL
1	F	415	ILE
1	F	430	ARG
1	F	432	ILE
1	F	446	LYS
1	F	449	ARG
1	F	461	LEU
1	F	463	ILE
1	F	468	ASN
1	F	470	GLU
1	F	481	SER
1	F	484	ASP
1	F	489	SER
1	F	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	242	HIS
1	A	243	GLN
1	A	380	HIS
1	A	458	HIS
1	B	72	ASN
1	B	242	HIS
1	B	243	GLN
1	B	380	HIS
1	B	433	HIS
1	B	458	HIS
1	C	242	HIS
1	C	243	GLN
1	C	308	GLN
1	C	309	ASN
1	C	380	HIS
1	C	431	ASN
1	C	458	HIS
1	D	242	HIS
1	D	243	GLN

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Mol	Chain	Res	Type
1	D	309	ASN
1	D	380	HIS
1	D	458	HIS
1	E	72	ASN
1	E	242	HIS
1	E	243	GLN
1	E	380	HIS
1	E	458	HIS
1	E	468	ASN
1	F	72	ASN
1	F	242	HIS
1	F	243	GLN
1	F	380	HIS
1	F	431	ASN
1	F	433	HIS
1	F	453	HIS
1	F	458	HIS
1	F	497	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	$\# Z > 2$
2	AHR	A	1503	2	8,9,10	0.68	0	11,13,14	1.90	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AHR	A	1504	2	8,9,10	0.63	0	11,13,14	1.65	3 (27%)
2	AHR	A	1505	2	10,10,10	1.55	1 (10%)	14,14,14	1.90	3 (21%)
4	AHR	B	1503	4	10,10,10	1.58	1 (10%)	14,14,14	1.95	3 (21%)
4	AHR	B	1504	4	8,9,10	0.62	0	11,13,14	1.69	3 (27%)
2	AHR	C	1503	2	10,10,10	1.58	1 (10%)	14,14,14	2.02	2 (14%)
2	AHR	C	1504	2	8,9,10	0.65	0	11,13,14	1.66	3 (27%)
2	AHR	C	1505	2	8,9,10	0.74	0	11,13,14	1.54	3 (27%)
2	AHR	D	1503	2	10,10,10	1.58	1 (10%)	14,14,14	2.06	2 (14%)
2	AHR	D	1504	2	8,9,10	0.69	0	11,13,14	1.64	3 (27%)
2	AHR	D	1505	2	8,9,10	0.73	0	11,13,14	1.70	3 (27%)
2	AHR	E	1503	2	10,10,10	1.60	1 (10%)	14,14,14	2.07	2 (14%)
2	AHR	E	1504	2	8,9,10	0.71	0	11,13,14	1.68	3 (27%)
2	AHR	E	1505	2	8,9,10	0.67	0	11,13,14	1.84	3 (27%)
4	AHR	F	1503	4	10,10,10	1.55	1 (10%)	14,14,14	1.93	3 (21%)
4	AHR	F	1504	4	8,9,10	0.68	0	11,13,14	1.69	3 (27%)

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	AHR	A	1503	2	-	0/0/16/18	0/1/1/1
2	AHR	A	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	A	1505	2	-	0/2/18/18	0/1/1/1
4	AHR	B	1503	4	-	0/2/18/18	0/1/1/1
4	AHR	B	1504	4	-	0/0/16/18	0/1/1/1
2	AHR	C	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	C	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	C	1505	2	-	0/0/16/18	0/1/1/1
2	AHR	D	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	D	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	D	1505	2	-	0/0/16/18	0/1/1/1
2	AHR	E	1503	2	-	0/2/18/18	0/1/1/1
2	AHR	E	1504	2	-	0/0/16/18	0/1/1/1
2	AHR	E	1505	2	-	0/0/16/18	0/1/1/1
4	AHR	F	1503	4	-	0/2/18/18	0/1/1/1
4	AHR	F	1504	4	-	0/0/16/18	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1505	AHR	O5'-C5'	-4.55	1.22	1.42
2	C	1503	AHR	O5'-C5'	-4.53	1.22	1.42
4	B	1503	AHR	O5'-C5'	-4.53	1.22	1.42
2	D	1503	AHR	O5'-C5'	-4.53	1.22	1.42
2	E	1503	AHR	O5'-C5'	-4.50	1.22	1.42
4	F	1503	AHR	O5'-C5'	-4.49	1.22	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1503	AHR	O1'-C1'-O4'	5.99	119.45	111.28
2	D	1503	AHR	O1'-C1'-O4'	5.91	119.34	111.28
2	C	1503	AHR	O1'-C1'-O4'	5.76	119.14	111.28
4	F	1503	AHR	O1'-C1'-O4'	5.18	118.34	111.28
4	B	1503	AHR	O1'-C1'-O4'	5.18	118.34	111.28
2	A	1505	AHR	O1'-C1'-O4'	4.99	118.08	111.28
2	A	1503	AHR	C2'-C3'-C4'	4.09	106.74	101.77
4	F	1504	AHR	C2'-C3'-C4'	3.70	106.27	101.77
2	C	1504	AHR	C2'-C3'-C4'	3.66	106.21	101.77
4	B	1504	AHR	C2'-C3'-C4'	3.62	106.16	101.77
2	D	1504	AHR	C2'-C3'-C4'	3.55	106.08	101.77
2	E	1505	AHR	C2'-C3'-C4'	3.54	106.07	101.77
2	E	1504	AHR	C2'-C3'-C4'	3.54	106.06	101.77
2	A	1504	AHR	C2'-C3'-C4'	3.44	105.95	101.77
2	E	1505	AHR	O4'-C1'-C2'	3.32	107.90	104.72
2	A	1503	AHR	O4'-C1'-C2'	3.23	107.82	104.72
4	F	1503	AHR	O5'-C5'-C4'	3.15	122.20	111.36
2	E	1503	AHR	O5'-C5'-C4'	3.14	122.16	111.36
2	D	1505	AHR	O4'-C1'-C2'	3.13	107.71	104.72
2	D	1503	AHR	O5'-C5'-C4'	3.12	122.08	111.36
4	B	1503	AHR	O5'-C5'-C4'	3.10	122.04	111.36
2	A	1505	AHR	O5'-C5'-C4'	3.07	121.91	111.36
2	C	1503	AHR	O5'-C5'-C4'	3.01	121.71	111.36
2	D	1505	AHR	C2'-C3'-C4'	2.93	105.33	101.77
2	D	1505	AHR	C1'-C2'-C3'	2.81	105.97	102.33
2	C	1505	AHR	C1'-C2'-C3'	2.81	105.97	102.33
2	A	1503	AHR	C1'-C2'-C3'	2.75	105.89	102.33
2	C	1505	AHR	O4'-C1'-C2'	2.73	107.34	104.72
2	D	1504	AHR	C1'-C2'-C3'	2.72	105.85	102.33
2	E	1504	AHR	C1'-C2'-C3'	2.67	105.79	102.33
2	E	1505	AHR	C1'-C2'-C3'	2.67	105.78	102.33
2	A	1504	AHR	O4'-C1'-C2'	2.62	107.23	104.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1504	AHR	C1'-C2'-C3'	2.58	105.67	102.33
4	F	1504	AHR	C1'-C2'-C3'	2.56	105.64	102.33
4	B	1504	AHR	O4'-C1'-C2'	2.52	107.13	104.72
2	A	1504	AHR	C1'-C2'-C3'	2.52	105.59	102.33
2	C	1504	AHR	C1'-C2'-C3'	2.48	105.54	102.33
2	C	1504	AHR	O4'-C1'-C2'	2.47	107.08	104.72
2	E	1504	AHR	O4'-C1'-C2'	2.44	107.06	104.72
4	F	1504	AHR	O4'-C1'-C2'	2.38	107.00	104.72
2	A	1505	AHR	C1'-C2'-C3'	2.36	105.38	102.33
2	C	1505	AHR	C2'-C3'-C4'	2.33	104.60	101.77
4	B	1503	AHR	C1'-C2'-C3'	2.29	105.29	102.33
2	D	1504	AHR	O4'-C1'-C2'	2.20	106.83	104.72
4	F	1503	AHR	C1'-C2'-C3'	2.09	105.03	102.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

9 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	EDO	A	1506	-	3,3,3	0.54	0	2,2,2	0.38	0
3	EDO	B	1505	-	3,3,3	0.59	0	2,2,2	0.25	0
3	EDO	B	1506	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	C	1506	-	3,3,3	0.53	0	2,2,2	0.40	0
3	EDO	D	1506	-	3,3,3	0.57	0	2,2,2	0.31	0
3	EDO	D	1507	-	3,3,3	0.54	0	2,2,2	0.39	0
3	EDO	E	1506	-	3,3,3	0.58	0	2,2,2	0.29	0
3	EDO	E	1507	-	3,3,3	0.64	0	2,2,2	0.46	0
3	EDO	F	1505	-	3,3,3	0.89	0	2,2,2	0.73	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
3	EDO	A	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1505	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1507	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1506	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1507	-	-	0/1/1/1	0/0/0/0
3	EDO	F	1505	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	496/513 (96%)	0.88	43 (8%)	10 10	23, 46, 46, 48	0
1	B	497/513 (96%)	0.82	40 (8%)	12 13	22, 46, 46, 47	0
1	C	496/513 (96%)	0.91	54 (10%)	6 6	22, 46, 46, 48	0
1	D	499/513 (97%)	0.90	37 (7%)	14 15	22, 46, 46, 47	0
1	E	492/513 (95%)	0.92	51 (10%)	7 7	23, 46, 46, 48	0
1	F	496/513 (96%)	0.87	47 (9%)	8 8	23, 46, 46, 48	0
All	All	2976/3078 (96%)	0.88	272 (9%)	9 9	22, 46, 46, 48	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	VAL	5.2
1	C	501	ILE	5.1
1	C	484	ASP	4.9
1	B	12	TYR	4.8
1	D	490	MET	4.8
1	A	484	ASP	4.8
1	F	484	ASP	4.3
1	E	436	ILE	4.3
1	E	487	LEU	4.3
1	E	439	VAL	4.3
1	A	416	TYR	4.1
1	D	488	THR	4.1
1	F	441	ASP	4.1
1	A	490	MET	4.0
1	A	482	PHE	4.0
1	B	410	ILE	4.0
1	C	483	ASP	4.0
1	F	481	SER	4.0
1	A	11	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	483	ASP	3.9
1	E	442	VAL	3.9
1	A	12	TYR	3.9
1	D	443	ARG	3.9
1	E	441	ASP	3.9
1	C	476	ASN	3.8
1	F	12	TYR	3.8
1	C	12	TYR	3.8
1	A	445	MET	3.7
1	B	438	LEU	3.7
1	F	486	ILE	3.7
1	E	11	ASP	3.7
1	B	3	LYS	3.6
1	A	476	ASN	3.6
1	D	368	ALA	3.6
1	D	12	TYR	3.6
1	A	398	LEU	3.6
1	E	490	MET	3.6
1	A	459	GLN	3.5
1	D	410	ILE	3.5
1	C	436	ILE	3.5
1	D	484	ASP	3.5
1	E	501	ILE	3.5
1	C	482	PHE	3.5
1	A	487	LEU	3.4
1	C	437	VAL	3.4
1	D	437	VAL	3.4
1	D	416	TYR	3.4
1	F	443	ARG	3.4
1	D	431	ASN	3.4
1	A	457	GLU	3.4
1	D	485	GLY	3.4
1	F	308	GLN	3.4
1	A	483	ASP	3.3
1	C	423	VAL	3.3
1	B	484	ASP	3.3
1	E	437	VAL	3.3
1	C	457	GLU	3.3
1	C	445	MET	3.3
1	F	437	VAL	3.3
1	C	490	MET	3.2
1	E	481	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	450	LEU	3.2
1	F	416	TYR	3.2
1	A	464	ARG	3.2
1	B	443	ARG	3.2
1	F	306	ILE	3.2
1	E	12	TYR	3.2
1	B	485	GLY	3.2
1	C	414	ALA	3.2
1	D	433	HIS	3.2
1	F	419	GLU	3.2
1	C	416	TYR	3.2
1	A	302	GLU	3.2
1	E	435	ASP	3.1
1	A	501	ILE	3.1
1	F	421	GLU	3.1
1	C	464	ARG	3.1
1	B	481	SER	3.1
1	B	302	GLU	3.1
1	B	431	ASN	3.1
1	E	4	ALA	3.1
1	D	41	GLY	3.0
1	F	410	ILE	3.0
1	B	487	LEU	3.0
1	F	310	GLU	3.0
1	D	11	ASP	3.0
1	A	408	THR	3.0
1	E	450	LEU	3.0
1	A	443	ARG	3.0
1	F	8	VAL	3.0
1	D	304	ALA	3.0
1	F	11	ASP	3.0
1	C	499	ILE	2.9
1	F	485	GLY	2.9
1	E	5	ARG	2.9
1	F	442	VAL	2.9
1	E	426	PHE	2.9
1	C	449	ARG	2.9
1	F	451	LEU	2.9
1	E	480	SER	2.9
1	E	48	ASP	2.9
1	D	367	GLY	2.9
1	C	438	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	469	GLY	2.9
1	B	483	ASP	2.9
1	E	40	PRO	2.9
1	A	485	GLY	2.9
1	C	487	LEU	2.9
1	C	480	SER	2.8
1	B	436	ILE	2.8
1	F	439	VAL	2.8
1	A	433	HIS	2.8
1	B	433	HIS	2.8
1	E	498	VAL	2.8
1	D	302	GLU	2.8
1	D	306	ILE	2.8
1	C	439	VAL	2.8
1	B	439	VAL	2.8
1	E	451	LEU	2.7
1	A	421	GLU	2.7
1	E	310	GLU	2.7
1	E	6	MET	2.7
1	C	178	TRP	2.7
1	A	367	GLY	2.7
1	E	9	ASP	2.7
1	D	246	GLY	2.7
1	B	490	MET	2.7
1	C	478	ASP	2.7
1	A	478	ASP	2.6
1	C	432	ILE	2.6
1	F	445	MET	2.6
1	C	442	VAL	2.6
1	B	308	GLN	2.6
1	B	441	ASP	2.6
1	D	468	ASN	2.6
1	A	444	GLY	2.6
1	D	432	ILE	2.6
1	D	436	ILE	2.6
1	F	14	ILE	2.6
1	C	11	ASP	2.6
1	A	5	ARG	2.6
1	A	436	ILE	2.6
1	C	459	GLN	2.6
1	D	487	LEU	2.6
1	E	431	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	485	GLY	2.5
1	B	399	HIS	2.5
1	A	368	ALA	2.5
1	A	430	ARG	2.5
1	B	4	ALA	2.5
1	A	431	ASN	2.5
1	B	461	LEU	2.5
1	C	394	ILE	2.5
1	B	478	ASP	2.5
1	D	467	VAL	2.5
1	B	301	ASN	2.5
1	E	432	ILE	2.5
1	E	488	THR	2.5
1	C	255	PHE	2.5
1	E	107	ILE	2.5
1	D	406	ASP	2.4
1	C	491	LEU	2.4
1	D	309	ASN	2.4
1	B	430	ARG	2.4
1	C	410	ILE	2.4
1	C	456	LEU	2.4
1	E	440	SER	2.4
1	A	502	GLY	2.4
1	B	434	GLU	2.4
1	A	394	ILE	2.4
1	E	155	ILE	2.4
1	A	392	PRO	2.4
1	F	392	PRO	2.4
1	E	47	GLU	2.4
1	B	8	VAL	2.4
1	E	472	VAL	2.4
1	D	185	MET	2.4
1	F	307	MET	2.4
1	E	434	GLU	2.3
1	C	492	ARG	2.3
1	C	486	ILE	2.3
1	F	414	ALA	2.3
1	C	325	PHE	2.3
1	B	456	LEU	2.3
1	D	446	LYS	2.3
1	F	41	GLY	2.3
1	A	439	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	5	ARG	2.3
1	E	308	GLN	2.3
1	C	495	SER	2.3
1	E	50	PHE	2.3
1	C	450	LEU	2.3
1	F	476	ASN	2.3
1	B	160	LYS	2.3
1	F	444	GLY	2.3
1	F	449	ARG	2.3
1	C	398	LEU	2.3
1	D	483	ASP	2.2
1	D	107	ILE	2.2
1	E	410	ILE	2.2
1	E	384	TYR	2.2
1	F	6	MET	2.2
1	E	305	ASN	2.2
1	F	394	ILE	2.2
1	A	475	LYS	2.2
1	E	85	PRO	2.2
1	B	246	GLY	2.2
1	D	155	ILE	2.2
1	A	493	ARG	2.2
1	E	476	ASN	2.2
1	C	397	PRO	2.2
1	F	3	LYS	2.2
1	B	442	VAL	2.2
1	F	304	ALA	2.2
1	E	14	ILE	2.2
1	E	499	ILE	2.2
1	F	501	ILE	2.2
1	C	309	ASN	2.1
1	A	428	VAL	2.1
1	E	369	ALA	2.1
1	B	499	ILE	2.1
1	E	454	ILE	2.1
1	A	304	ALA	2.1
1	A	236	VAL	2.1
1	F	222	PRO	2.1
1	A	477	SER	2.1
1	C	5	ARG	2.1
1	E	3	LYS	2.1
1	E	500	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	409	ASP	2.1
1	C	329	LEU	2.1
1	D	459	GLN	2.1
1	B	304	ALA	2.1
1	A	455	VAL	2.1
1	C	8	VAL	2.1
1	E	87	GLU	2.1
1	F	500	ARG	2.1
1	F	482	PHE	2.1
1	B	459	GLN	2.1
1	B	368	ALA	2.1
1	C	493	ARG	2.1
1	E	478	ASP	2.1
1	D	461	LEU	2.1
1	E	112	LYS	2.1
1	C	304	ALA	2.1
1	A	228	VAL	2.1
1	B	211	CYS	2.1
1	B	397	PRO	2.1
1	B	480	SER	2.1
1	F	478	ASP	2.1
1	F	365	ASN	2.1
1	C	477	SER	2.1
1	A	14	ILE	2.1
1	F	47	GLU	2.1
1	F	434	GLU	2.1
1	A	196	ALA	2.1
1	F	9	ASP	2.1
1	D	418	GLU	2.1
1	E	390	LEU	2.1
1	F	309	ASN	2.1
1	C	393	VAL	2.0
1	D	325	PHE	2.0
1	D	448	TYR	2.0
1	F	7	THR	2.0
1	C	303	ASP	2.0
1	C	308	GLN	2.0
1	C	422	GLU	2.0
1	C	368	ALA	2.0
1	D	4	ALA	2.0
1	C	472	VAL	2.0
1	E	423	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	384	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	AHR	B	1504	9/10	0.34	6.50	46,46,47,48	0
2	AHR	A	1504	9/10	0.37	3.83	46,46,47,48	0
2	AHR	D	1504	9/10	0.27	2.89	46,46,47,48	0
2	AHR	E	1504	9/10	0.26	2.37	46,46,47,48	0
4	AHR	B	1503	10/10	0.26	1.72	46,46,46,46	0
2	AHR	D	1503	10/10	0.24	1.21	46,46,46,46	0
2	AHR	C	1504	9/10	0.28	0.94	46,46,47,48	0
2	AHR	A	1505	10/10	0.26	0.83	45,46,46,46	0
4	AHR	F	1504	9/10	0.25	0.76	46,46,47,48	0
2	AHR	E	1503	10/10	0.23	0.65	45,46,46,46	0
2	AHR	C	1503	10/10	0.23	0.05	46,46,46,46	0
4	AHR	F	1503	10/10	0.20	-0.77	46,46,46,46	0
2	AHR	C	1505	9/10	0.54	-	52,56,57,57	0
2	AHR	D	1505	9/10	0.50	-	52,56,57,57	0
2	AHR	A	1503	9/10	0.49	-	53,57,58,58	0
2	AHR	E	1505	9/10	0.38	-	52,55,55,55	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	E	1506	4/4	0.45	10.58	52,52,52,53	0
3	EDO	B	1505	4/4	0.47	6.87	54,54,55,55	0
3	EDO	D	1507	4/4	0.29	4.03	66,66,66,66	0
3	EDO	D	1506	4/4	0.34	3.64	47,47,47,48	0
3	EDO	B	1506	4/4	0.23	0.69	57,57,57,57	0
3	EDO	F	1505	4/4	0.22	0.27	62,62,63,63	0
3	EDO	C	1506	4/4	0.18	-1.56	51,51,51,51	0
3	EDO	A	1506	4/4	0.15	-2.24	50,50,50,50	0
3	EDO	E	1507	4/4	0.12	-2.66	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.