Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2022 – 12:10 pm GMT

PDB ID	:	6G9E
Title	:	Crystal structure of immunomodulatory active chitinase from Trichuris suis - TsES1 - 6 molecules in ASU
Authors	:	Malecki, P.H.; Balster, K.; Hartmann, S.; Weiss, M.S.; Heinemann, U.
Deposited on	:	2018-04-10
Resolution	:	2.69 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

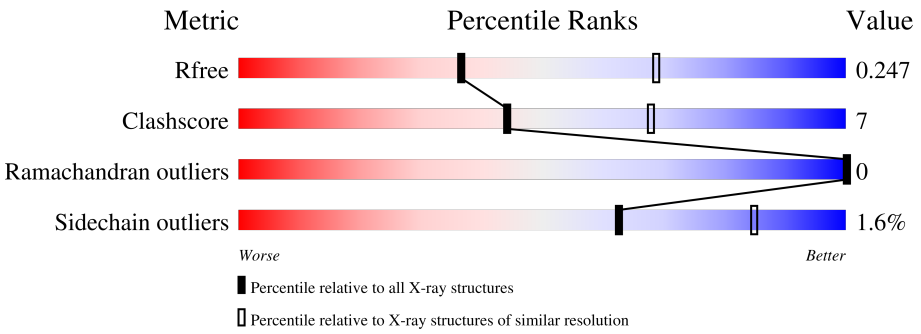
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	495	61% 13% 26%
1	B	495	61% 13% 26%
1	C	495	62% 13% 26%
1	D	495	62% 12% 26%
1	E	495	60% 14% 26%
1	F	495	64% 10% 26%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18247 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 Immunomodulatory active chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2962	1904	475	569	14	0	0	0
1	B	368	2962	1904	475	569	14	0	0	0
1	C	368	2962	1904	475	569	14	0	0	0
1	D	368	2962	1904	475	569	14	0	0	0
1	E	368	2962	1904	475	569	14	0	0	0
1	F	368	2962	1904	475	569	14	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	THR	-	expression tag	UNP A0A085LU44
A	490	HIS	-	expression tag	UNP A0A085LU44
A	491	HIS	-	expression tag	UNP A0A085LU44
A	492	HIS	-	expression tag	UNP A0A085LU44
A	493	HIS	-	expression tag	UNP A0A085LU44
A	494	HIS	-	expression tag	UNP A0A085LU44
A	495	HIS	-	expression tag	UNP A0A085LU44
B	489	THR	-	expression tag	UNP A0A085LU44
B	490	HIS	-	expression tag	UNP A0A085LU44
B	491	HIS	-	expression tag	UNP A0A085LU44
B	492	HIS	-	expression tag	UNP A0A085LU44
B	493	HIS	-	expression tag	UNP A0A085LU44
B	494	HIS	-	expression tag	UNP A0A085LU44
B	495	HIS	-	expression tag	UNP A0A085LU44
C	489	THR	-	expression tag	UNP A0A085LU44
C	490	HIS	-	expression tag	UNP A0A085LU44
C	491	HIS	-	expression tag	UNP A0A085LU44

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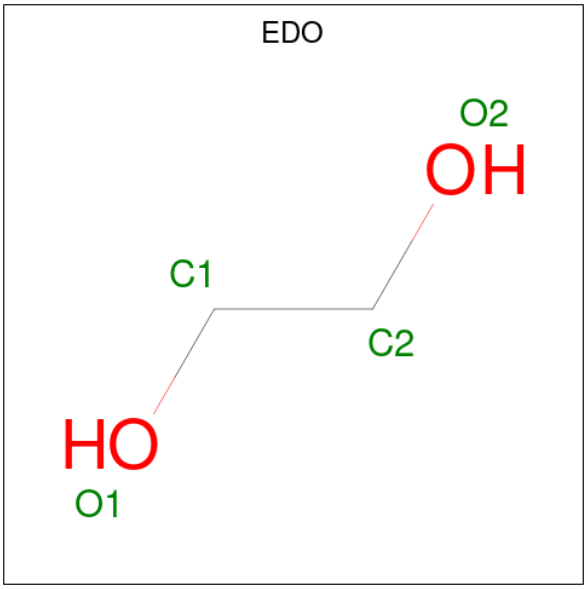
Chain	Residue	Modelled	Actual	Comment	Reference
C	492	HIS	-	expression tag	UNP A0A085LU44
C	493	HIS	-	expression tag	UNP A0A085LU44
C	494	HIS	-	expression tag	UNP A0A085LU44
C	495	HIS	-	expression tag	UNP A0A085LU44
D	489	THR	-	expression tag	UNP A0A085LU44
D	490	HIS	-	expression tag	UNP A0A085LU44
D	491	HIS	-	expression tag	UNP A0A085LU44
D	492	HIS	-	expression tag	UNP A0A085LU44
D	493	HIS	-	expression tag	UNP A0A085LU44
D	494	HIS	-	expression tag	UNP A0A085LU44
D	495	HIS	-	expression tag	UNP A0A085LU44
E	489	THR	-	expression tag	UNP A0A085LU44
E	490	HIS	-	expression tag	UNP A0A085LU44
E	491	HIS	-	expression tag	UNP A0A085LU44
E	492	HIS	-	expression tag	UNP A0A085LU44
E	493	HIS	-	expression tag	UNP A0A085LU44
E	494	HIS	-	expression tag	UNP A0A085LU44
E	495	HIS	-	expression tag	UNP A0A085LU44
F	489	THR	-	expression tag	UNP A0A085LU44
F	490	HIS	-	expression tag	UNP A0A085LU44
F	491	HIS	-	expression tag	UNP A0A085LU44
F	492	HIS	-	expression tag	UNP A0A085LU44
F	493	HIS	-	expression tag	UNP A0A085LU44
F	494	HIS	-	expression tag	UNP A0A085LU44
F	495	HIS	-	expression tag	UNP A0A085LU44

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 3 is water.

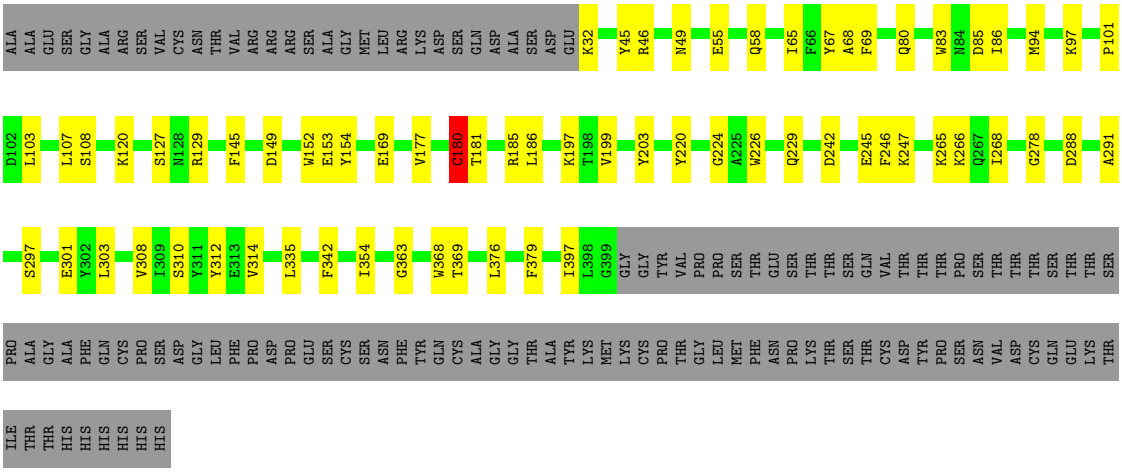
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	98	99	99	0	1
3	B	104	104	104	0	0
3	C	98	98	98	0	0
3	D	47	47	47	0	0
3	E	56	56	56	0	0
3	F	50	51	51	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

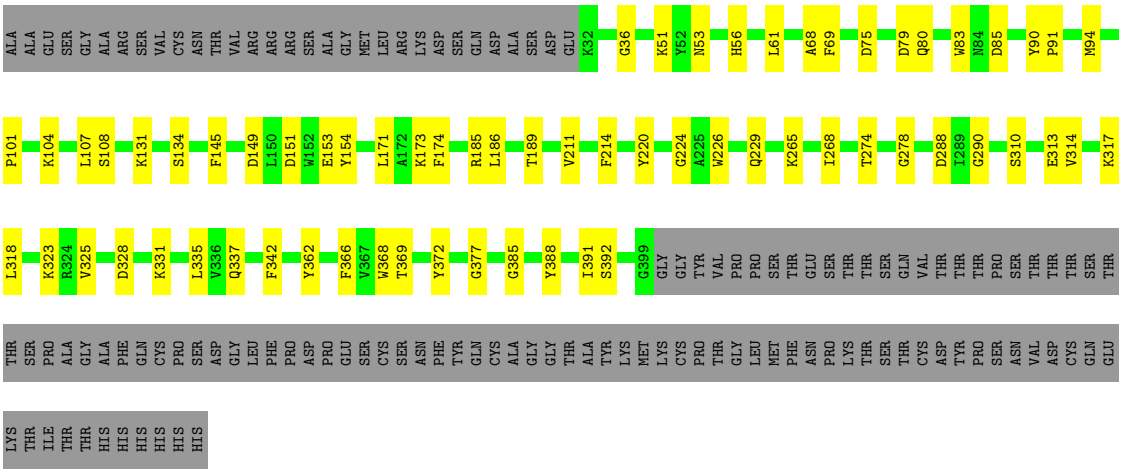
- Molecule 1: Immunomodulatory active chitinase

Chain A: 61% 13% 26%



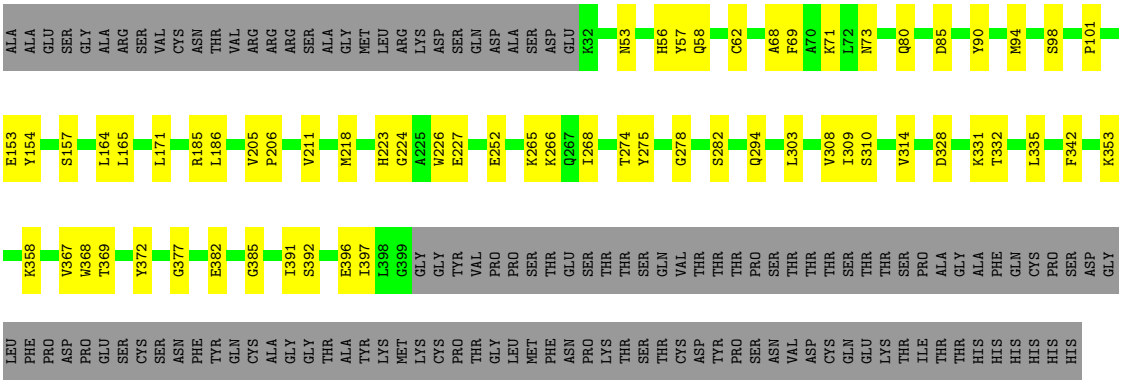
- Molecule 1: Immunomodulatory active chitinase

Chain B: 61% 13% 26%



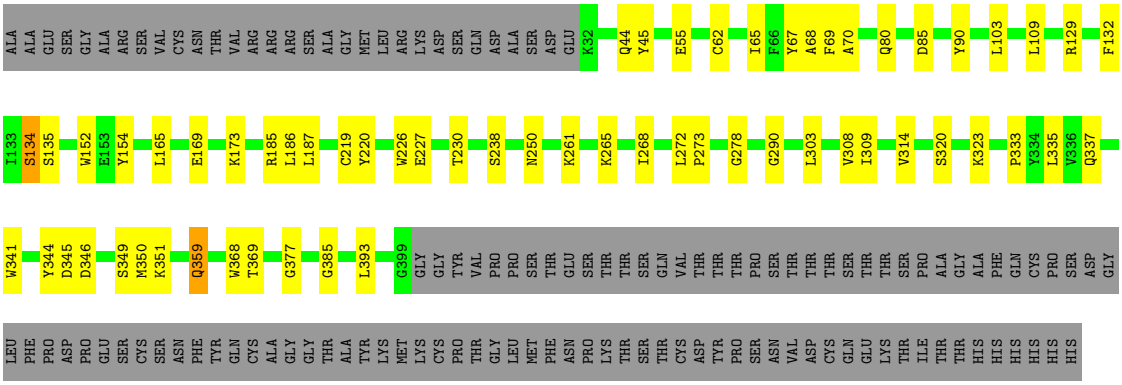
- Molecule 1: Immunomodulatory active chitinase

Chain C: 62% 13% 26%



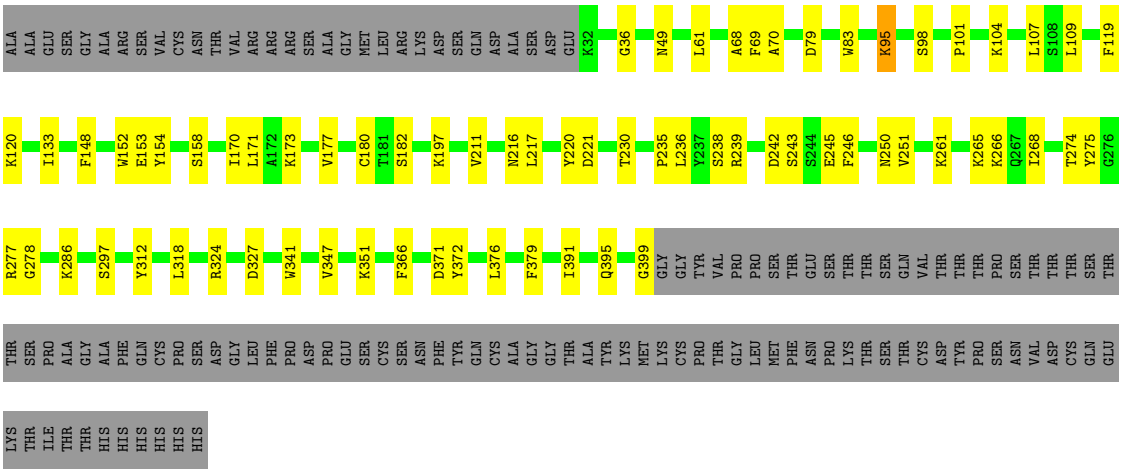
- Molecule 1: Immunomodulatory active chitinase

Chain D:



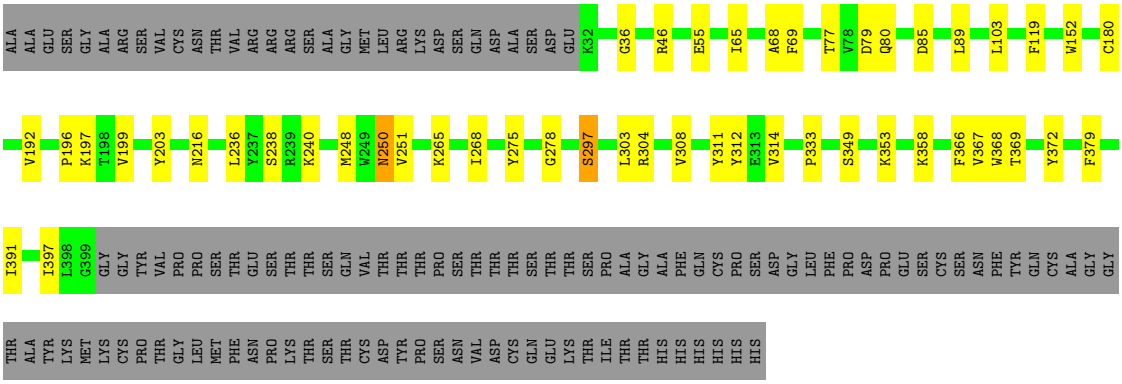
- Molecule 1: Immunomodulatory active chitinase

Chain E:



- Molecule 1: Immunomodulatory active chitinase

Chain F:


ALA ALA GLU SER GLY ALA ARG SER VAL CYS ASN THR VAL ARG ARG ARG SER ALA GLY MET LEU ARG LYS ASP SER GLN ASP ALA SER ASP GLU K32 G36 R46 E55 I65 A68 F69 T77 V78 D79 Q80 D85 L89 L103 F119 W152 C180
V192 P196 K197 T198 V199 Y203 N216 L236 Y237 S238 R239 K240 M248 W249 N250 V251 K265 I268 Y275 G278 S297 L303 R304 V308 Y311 Y312 E313 V314 P333 S349 K353 K358 F366 V367 W368 T369 Y372 F379
I391 I397 L398 G399 GLY GLY TYR VAL PRO PRO SER THR GLU SER THR THR SER GLN VAL THR THR THR PRO SER THR THR THR SER THR THR SER PRO ALA GLY ALA PHE GLN CYS PRO SER ASP GLY LEU PHE PRO ASP PRO GLU SER CYS SER ASN PHE TYR GLN CYS ALA GLY GLY
THR ALA TYR LYS MET LYS CYS PRO THR GLY LEU MET PHE ASN PRO LYS THR SER THR CYS ASP TYR PRO SER ASN VAL ASP CYS GLN GLU LYS THR ILE THR THR HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	220.06Å 172.62Å 138.56Å 90.00° 128.41° 90.00°	Depositor
Resolution (Å)	45.61 – 2.69 45.61 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.61-2.69) 98.9 (45.61-2.69)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.249 0.194 , 0.247	Depositor DCC
R_{free} test set	1104 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.851	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.001 for k+l,h+l,-l 0.002 for -k+l,-h-l,-l 0.017 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18247	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.47	1/3044 (0.0%)	0.60	0/4126
1	B	0.48	0/3044	0.58	0/4126
1	C	0.47	0/3044	0.60	0/4126
1	D	0.46	0/3044	0.57	0/4126
1	E	0.46	1/3044 (0.0%)	0.57	0/4126
1	F	0.46	0/3044	0.58	0/4126
All	All	0.46	2/18264 (0.0%)	0.59	0/24756

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	CYS	CB-SG	-6.73	1.70	1.82
1	E	180	CYS	CB-SG	-5.05	1.73	1.81

There are no bond angle outliers.

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	2962	0	2823	47	0
1	B	2962	0	2823	42	0
1	C	2962	0	2823	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2962	0	2824	37	1
1	E	2962	0	2824	44	1
1	F	2962	0	2823	31	0
2	A	4	0	6	3	0
2	B	4	0	6	0	0
2	C	8	0	12	2	0
2	D	4	0	6	0	0
3	A	99	0	0	2	0
3	B	104	0	0	0	0
3	C	98	0	0	2	0
3	D	47	0	0	0	0
3	E	56	0	0	1	0
3	F	51	0	0	1	0
All	All	18247	0	16970	229	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:THR:HG22	1:C:353:LYS:HZ1	1.46	0.79
1:A:177:VAL:O	1:A:181:THR:HG22	1.82	0.79
1:A:46:ARG:HE	2:A:501:EDO:H12	1.51	0.76
1:D:165:LEU:O	1:D:169:GLU:HG3	1.86	0.75
1:B:323:LYS:HE2	1:B:325:VAL:HG22	1.72	0.71
1:A:80:GLN:NE2	1:A:86:ILE:H	1.90	0.69
1:C:282:SER:HA	1:C:294:GLN:HG3	1.75	0.68
1:C:223:HIS:HD2	1:C:227:GLU:OE2	1.79	0.65
1:C:164:LEU:HD23	2:C:502:EDO:H12	1.77	0.64
1:F:311:TYR:O	1:F:314:VAL:HG22	1.97	0.64
1:A:180:CYS:SG	1:F:180:CYS:CB	2.86	0.62
1:C:332:THR:HG22	1:C:353:LYS:NZ	2.15	0.60
1:F:367:VAL:HG11	1:F:391:ILE:HG12	1.84	0.60
1:F:65:ILE:HG13	1:F:103:LEU:HD11	1.83	0.60
1:E:153:GLU:HA	1:E:154:TYR:CD1	2.37	0.59
1:C:80:GLN:HB2	1:C:85:ASP:HB2	1.83	0.59
1:B:377:GLY:O	1:B:385:GLY:HA2	2.03	0.59
1:A:265:LYS:HA	1:A:268:ILE:HD12	1.85	0.58
1:D:265:LYS:HA	1:D:268:ILE:HD12	1.84	0.58
1:D:55:GLU:CD	1:D:55:GLU:H	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:HB2	1:A:247:LYS:HE2	1.83	0.58
1:B:83:TRP:HZ2	1:D:134:SER:HB3	1.68	0.57
1:B:75:ASP:O	1:B:131:LYS:HE2	2.04	0.57
1:A:46:ARG:NE	2:A:501:EDO:H12	2.18	0.56
1:E:235:PRO:O	1:E:251:VAL:HG23	2.06	0.56
1:C:392:SER:O	1:C:396:GLU:HG3	2.05	0.55
1:C:265:LYS:HA	1:C:268:ILE:HD12	1.88	0.55
1:D:185:ARG:HD2	1:D:186:LEU:O	2.07	0.55
1:D:129:ARG:NE	1:D:169:GLU:OE1	2.37	0.54
1:E:230:THR:HG23	1:E:341:TRP:CZ3	2.42	0.54
1:A:32:LYS:O	1:A:266:LYS:HE2	2.07	0.54
1:A:80:GLN:HE22	1:A:86:ILE:H	1.56	0.54
1:C:328:ASP:O	1:C:331:LYS:HE2	2.08	0.54
1:F:236:LEU:HD13	1:F:353:LYS:HG2	1.90	0.54
1:B:107:LEU:HD13	1:B:145:PHE:CZ	2.43	0.54
1:C:101:PRO:HG3	1:E:101:PRO:HG2	1.90	0.54
1:E:36:GLY:O	1:E:366:PHE:HA	2.09	0.53
1:D:70:ALA:HB3	1:D:109:LEU:HD13	1.90	0.53
1:E:395:GLN:HE22	1:E:399:GLY:HA3	1.73	0.53
1:E:395:GLN:O	1:E:395:GLN:NE2	2.38	0.53
1:A:278:GLY:C	1:A:297:SER:HB3	2.30	0.52
1:E:133:ILE:HG12	1:E:170:ILE:HG12	1.90	0.52
1:F:333:PRO:HD3	1:F:349:SER:HB3	1.91	0.52
1:F:265:LYS:HA	1:F:268:ILE:HD12	1.92	0.52
1:B:185:ARG:HG2	1:B:186:LEU:O	2.10	0.52
1:B:265:LYS:HE2	1:B:362:TYR:CZ	2.44	0.52
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.75	0.51
1:B:229:GLN:HG3	1:B:290:GLY:HA2	1.92	0.51
1:C:382:GLU:HB2	3:C:663:HOH:O	2.10	0.51
1:E:83:TRP:HB3	1:F:77:THR:HG21	1.92	0.51
1:E:324:ARG:HD3	3:E:526:HOH:O	2.11	0.51
1:F:236:LEU:HD12	1:F:251:VAL:HB	1.93	0.51
1:D:272:LEU:HB3	1:D:350:MET:CE	2.40	0.51
1:D:346:ASP:O	1:D:350:MET:HG3	2.10	0.51
1:A:83:TRP:HZ2	1:B:134:SER:HB3	1.76	0.50
1:E:243:SER:OG	1:E:245:GLU:HG2	2.12	0.50
1:A:46:ARG:HE	2:A:501:EDO:C1	2.22	0.50
1:C:223:HIS:HE1	3:C:640:HOH:O	1.95	0.50
1:D:351:LYS:HG3	1:D:393:LEU:HD13	1.94	0.50
1:F:358:LYS:HE2	1:F:397:ILE:O	2.12	0.50
1:B:388:TYR:O	1:B:392:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD13	1:A:145:PHE:CZ	2.47	0.49
1:B:51:LYS:HE2	1:B:53:ASN:HD21	1.78	0.49
1:A:49:ASN:HB3	1:A:376:LEU:HD11	1.93	0.49
1:E:238:SER:HB3	1:E:250:ASN:ND2	2.28	0.49
1:F:278:GLY:C	1:F:297:SER:HB3	2.34	0.49
1:A:153:GLU:HA	1:A:154:TYR:CD1	2.48	0.48
1:B:310:SER:OG	1:B:313:GLU:HG3	2.13	0.48
1:B:90:TYR:HB2	1:B:91:PRO:HD3	1.95	0.48
1:C:358:LYS:HE2	1:C:397:ILE:O	2.13	0.48
1:E:70:ALA:HB2	1:E:107:LEU:HD11	1.95	0.48
1:A:120:LYS:HE2	3:A:610:HOH:O	2.12	0.48
1:B:80:GLN:HB2	1:B:85:ASP:HB2	1.94	0.48
1:F:216:ASN:HB3	1:F:366:PHE:CE1	2.48	0.48
1:F:275:TYR:HB3	1:F:372:TYR:CD2	2.48	0.48
1:B:174:PHE:HB3	1:B:185:ARG:HG3	1.96	0.48
1:E:119:PHE:HB3	1:E:152:TRP:CE2	2.48	0.48
1:B:317:LYS:HD3	1:B:337:GLN:NE2	2.29	0.48
1:A:303:LEU:HD21	1:A:310:SER:HB3	1.96	0.48
1:A:185:ARG:HG2	1:A:185:ARG:NH1	2.27	0.47
1:F:303:LEU:HD12	1:F:308:VAL:HG12	1.96	0.47
1:D:173:LYS:HA	1:D:173:LYS:HD2	1.70	0.47
1:D:272:LEU:HB3	1:D:350:MET:HE1	1.97	0.47
1:A:224:GLY:HA3	1:A:226:TRP:CZ3	2.48	0.47
1:B:328:ASP:O	1:B:331:LYS:HE2	2.15	0.47
1:C:303:LEU:HD11	1:C:310:SER:HB3	1.97	0.47
1:F:36:GLY:O	1:F:366:PHE:HA	2.15	0.47
1:A:55:GLU:H	1:A:55:GLU:CD	2.18	0.47
1:C:154:TYR:HE1	1:C:218:MET:CE	2.28	0.47
1:C:223:HIS:CD2	1:C:227:GLU:OE2	2.65	0.47
1:C:278:GLY:HA3	1:C:342:PHE:CD1	2.50	0.47
1:E:275:TYR:HB3	1:E:372:TYR:CD2	2.50	0.47
1:D:68:ALA:HA	1:D:69:PHE:HA	1.69	0.47
1:E:120:LYS:NZ	1:E:158:SER:OG	2.46	0.47
1:A:266:LYS:HE3	1:A:363:GLY:HA2	1.97	0.47
1:B:151:ASP:O	1:B:153:GLU:HG3	2.14	0.47
1:B:36:GLY:O	1:B:366:PHE:HA	2.15	0.46
1:C:153:GLU:HA	1:C:154:TYR:CD1	2.50	0.46
1:D:226:TRP:CD1	1:D:227:GLU:HG3	2.50	0.46
1:F:368:TRP:HA	1:F:369:THR:HA	1.78	0.46
1:C:224:GLY:HA3	1:C:226:TRP:CZ3	2.51	0.46
1:A:80:GLN:HE21	1:A:85:ASP:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:LYS:O	1:D:335:LEU:HD12	2.15	0.46
1:E:245:GLU:HG3	1:E:246:PHE:CD2	2.50	0.46
1:F:46:ARG:NH1	3:F:502:HOH:O	2.42	0.46
1:D:320:SER:HB2	1:D:337:GLN:HE22	1.81	0.46
1:B:171:LEU:HD22	1:B:211:VAL:HA	1.98	0.46
1:D:368:TRP:HA	1:D:369:THR:HA	1.73	0.46
1:F:238:SER:HB3	1:F:250:ASN:HD21	1.80	0.46
1:B:90:TYR:O	1:B:94:MET:HG2	2.15	0.45
1:B:224:GLY:HA3	1:B:226:TRP:CH2	2.52	0.45
1:E:61:LEU:HG	1:E:391:ILE:HG22	1.98	0.45
1:E:49:ASN:HB3	1:E:376:LEU:HD11	1.97	0.45
1:C:71:LYS:HE3	1:C:73:ASN:OD1	2.17	0.45
1:E:265:LYS:HA	1:E:268:ILE:HD12	1.99	0.45
1:A:301:GLU:HG2	3:A:649:HOH:O	2.17	0.45
1:B:368:TRP:CD2	1:B:369:THR:HG22	2.52	0.45
1:E:347:VAL:O	1:E:351:LYS:HG3	2.16	0.45
1:F:68:ALA:HA	1:F:69:PHE:HA	1.80	0.45
1:A:180:CYS:SG	1:F:180:CYS:HA	2.56	0.45
1:C:205:VAL:HB	1:C:206:PRO:HD3	1.99	0.45
1:A:49:ASN:HB3	1:A:376:LEU:CD1	2.47	0.44
1:C:53:ASN:O	1:C:56:HIS:HB2	2.17	0.44
1:B:314:VAL:HG13	1:B:335:LEU:HD22	2.00	0.44
1:D:80:GLN:HB2	1:D:85:ASP:HB2	1.99	0.44
1:C:275:TYR:HB3	1:C:372:TYR:CD2	2.53	0.44
1:E:95:LYS:HE2	1:E:98:SER:HB3	2.00	0.44
1:A:368:TRP:HA	1:A:369:THR:HA	1.82	0.44
1:C:185:ARG:HD2	1:C:186:LEU:O	2.18	0.44
1:E:312:TYR:HB2	1:E:379:PHE:CG	2.53	0.44
1:B:189:THR:HG21	1:B:214:PHE:CE1	2.51	0.44
1:C:57:TYR:CG	1:C:58:GLN:N	2.86	0.44
1:C:165:LEU:HG	2:C:502:EDO:H22	1.99	0.44
1:F:55:GLU:H	1:F:55:GLU:CD	2.19	0.44
1:C:68:ALA:HA	1:C:69:PHE:HA	1.81	0.43
1:A:314:VAL:HG13	1:A:335:LEU:HD22	2.00	0.43
1:C:314:VAL:HG13	1:C:335:LEU:HD22	2.01	0.43
1:E:230:THR:HG23	1:E:341:TRP:CH2	2.53	0.43
1:B:61:LEU:HG	1:B:391:ILE:HG22	2.00	0.43
1:D:309:ILE:HG12	1:D:314:VAL:HG23	2.00	0.43
1:A:65:ILE:HD12	1:A:103:LEU:HD21	2.01	0.43
1:A:245:GLU:HG3	1:A:246:PHE:CD2	2.54	0.43
1:C:98:SER:O	1:E:101:PRO:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ILE:HD12	1:D:103:LEU:HD21	2.01	0.43
1:B:274:THR:OG1	1:B:372:TYR:HB2	2.18	0.43
1:D:377:GLY:O	1:D:385:GLY:HA2	2.18	0.43
1:E:104:LYS:HB2	1:E:104:LYS:HE2	1.77	0.43
1:E:239:ARG:NH1	1:E:327:ASP:OD2	2.52	0.43
1:E:266:LYS:HD2	1:E:266:LYS:HA	1.75	0.43
1:A:278:GLY:HA3	1:A:342:PHE:CD1	2.54	0.43
1:B:278:GLY:HA3	1:B:342:PHE:CD1	2.54	0.43
1:B:68:ALA:HA	1:B:69:PHE:HA	1.81	0.43
1:E:197:LYS:HA	1:E:197:LYS:HD3	1.74	0.43
1:A:68:ALA:HA	1:A:69:PHE:HA	1.67	0.42
1:C:90:TYR:O	1:C:94:MET:HG2	2.19	0.42
1:E:278:GLY:C	1:E:297:SER:HB3	2.39	0.42
1:C:367:VAL:HG11	1:C:391:ILE:HG12	2.01	0.42
1:D:67:TYR:CE1	1:D:90:TYR:HE1	2.37	0.42
1:D:278:GLY:HA2	1:D:341:TRP:O	2.20	0.42
1:A:303:LEU:HD12	1:A:308:VAL:HG12	2.00	0.42
1:E:395:GLN:HE21	1:E:395:GLN:C	2.20	0.42
1:F:304:ARG:HH11	1:F:304:ARG:HD3	1.65	0.42
1:D:44:GLN:HG3	1:D:45:TYR:CD1	2.54	0.42
1:E:318:LEU:HD23	1:E:318:LEU:HA	1.88	0.42
1:C:308:VAL:HG12	1:C:309:ILE:N	2.34	0.42
1:A:288:ASP:H	1:A:291:ALA:HB2	1.84	0.42
1:B:153:GLU:HA	1:B:154:TYR:CD1	2.55	0.42
1:A:129:ARG:NH2	1:A:169:GLU:OE2	2.49	0.42
1:C:266:LYS:HD2	1:C:266:LYS:HA	1.75	0.42
1:F:199:VAL:HA	1:F:203:TYR:HD1	1.85	0.42
1:D:368:TRP:CD2	1:D:369:THR:HG22	2.55	0.42
1:E:68:ALA:HA	1:E:69:PHE:HA	1.71	0.42
1:E:274:THR:OG1	1:E:372:TYR:HB2	2.19	0.42
1:F:85:ASP:HA	1:F:89:LEU:HB2	2.00	0.42
1:A:45:TYR:CE1	1:B:131:LYS:HA	2.54	0.42
1:A:101:PRO:HG2	1:E:101:PRO:HG2	2.02	0.42
1:B:53:ASN:O	1:B:56:HIS:HB2	2.20	0.42
1:B:173:LYS:HA	1:B:173:LYS:HD3	1.77	0.42
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.93	0.42
1:A:185:ARG:NH1	1:A:186:LEU:O	2.53	0.41
1:C:377:GLY:O	1:C:385:GLY:HA2	2.20	0.41
1:E:173:LYS:O	1:E:177:VAL:HG23	2.20	0.41
1:E:217:LEU:HD12	1:E:217:LEU:HA	1.87	0.41
1:E:395:GLN:NE2	1:E:399:GLY:HA3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:TYR:O	1:A:108:SER:HB2	2.20	0.41
1:B:61:LEU:HD21	1:B:388:TYR:CG	2.55	0.41
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.84	0.41
1:B:83:TRP:CZ2	1:D:134:SER:HB3	2.53	0.41
1:C:171:LEU:HD22	1:C:211:VAL:HA	2.02	0.41
1:D:132:PHE:O	1:D:135:SER:HB3	2.19	0.41
1:B:108:SER:HA	1:B:149:ASP:O	2.20	0.41
1:C:274:THR:OG1	1:C:372:TYR:HB2	2.20	0.41
1:D:303:LEU:HD12	1:D:308:VAL:HG12	2.02	0.41
1:D:314:VAL:HG11	1:D:344:TYR:CE2	2.56	0.41
1:E:109:LEU:HB2	1:E:148:PHE:HE1	1.86	0.41
1:E:221:ASP:OD1	1:E:277:ARG:NH2	2.52	0.41
1:F:192:VAL:HG12	1:F:203:TYR:CE2	2.55	0.41
1:F:368:TRP:CD2	1:F:369:THR:HG22	2.56	0.41
1:A:199:VAL:HA	1:A:203:TYR:HD1	1.85	0.41
1:C:223:HIS:HB3	1:C:227:GLU:OE1	2.21	0.41
1:D:109:LEU:HD12	1:D:109:LEU:HA	1.91	0.41
1:F:89:LEU:HD23	1:F:89:LEU:HA	1.70	0.41
1:A:199:VAL:HA	1:A:203:TYR:CD1	2.55	0.41
1:A:152:TRP:O	1:A:154:TYR:HA	2.21	0.41
1:D:152:TRP:CD1	1:D:152:TRP:C	2.92	0.41
1:D:152:TRP:O	1:D:154:TYR:HA	2.21	0.41
1:D:230:THR:OG1	1:D:290:GLY:N	2.52	0.41
1:A:354:ILE:HG21	1:A:397:ILE:HB	2.02	0.41
1:B:265:LYS:HA	1:B:268:ILE:HD12	2.03	0.41
1:D:238:SER:HB3	1:D:250:ASN:ND2	2.35	0.41
1:E:236:LEU:HD12	1:E:251:VAL:HB	2.03	0.41
1:E:239:ARG:O	1:E:242:ASP:HB2	2.21	0.41
1:F:80:GLN:HB2	1:F:85:ASP:HB2	2.03	0.41
1:A:108:SER:OG	1:A:149:ASP:HB3	2.21	0.41
1:D:273:PRO:HG2	1:D:345:ASP:OD1	2.20	0.40
1:D:333:PRO:HD3	1:D:349:SER:HB3	2.02	0.40
1:E:216:ASN:HB3	1:E:366:PHE:CE2	2.56	0.40
1:F:312:TYR:HB2	1:F:379:PHE:CB	2.51	0.40
1:B:368:TRP:HA	1:B:369:THR:HA	1.74	0.40
1:A:312:TYR:HB2	1:A:379:PHE:CB	2.51	0.40
1:D:187:LEU:HD23	1:D:187:LEU:HA	1.84	0.40
1:A:83:TRP:CZ2	1:B:134:SER:HB3	2.55	0.40
1:C:368:TRP:HA	1:C:369:THR:HA	1.81	0.40
1:F:119:PHE:HB3	1:F:152:TRP:CE2	2.57	0.40
1:A:94:MET:O	1:A:97:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:HD21	1:B:388:TYR:CD1	2.57	0.40
1:C:154:TYR:HE1	1:C:218:MET:HE1	1.86	0.40
1:E:171:LEU:HD22	1:E:211:VAL:HA	2.04	0.40
1:F:196:PRO:HG2	1:F:248:MET:HB3	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:GLN:OE1	1:E:286:LYS:NZ[4_648]	2.05	0.15

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	366/495 (74%)	348 (95%)	18 (5%)	0	100	100
1	B	366/495 (74%)	358 (98%)	8 (2%)	0	100	100
1	C	366/495 (74%)	353 (96%)	13 (4%)	0	100	100
1	D	366/495 (74%)	356 (97%)	10 (3%)	0	100	100
1	E	366/495 (74%)	349 (95%)	17 (5%)	0	100	100
1	F	366/495 (74%)	353 (96%)	13 (4%)	0	100	100
All	All	2196/2970 (74%)	2117 (96%)	79 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/426 (74%)	311 (98%)	6 (2%)	57	82
1	B	317/426 (74%)	312 (98%)	5 (2%)	62	85
1	C	317/426 (74%)	314 (99%)	3 (1%)	78	92
1	D	317/426 (74%)	311 (98%)	6 (2%)	57	82
1	E	317/426 (74%)	311 (98%)	6 (2%)	57	82
1	F	317/426 (74%)	312 (98%)	5 (2%)	62	85
All	All	1902/2556 (74%)	1871 (98%)	31 (2%)	62	85

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	127	SER
1	A	180	CYS
1	A	197	LYS
1	A	220	TYR
1	A	229	GLN
1	B	79	ASP
1	B	101	PRO
1	B	104	LYS
1	B	220	TYR
1	B	288	ASP
1	C	62	CYS
1	C	157	SER
1	C	252	GLU
1	D	62	CYS
1	D	134	SER
1	D	219	CYS
1	D	220	TYR
1	D	261	LYS
1	D	359	GLN
1	E	79	ASP
1	E	95	LYS
1	E	182	SER
1	E	220	TYR
1	E	261	LYS
1	E	371	ASP
1	F	79	ASP

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Mol	Chain	Res	Type
1	F	197	LYS
1	F	240	LYS
1	F	250	ASN
1	F	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	C	223	HIS
1	E	395	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
2	EDO	D	501	-	3,3,3	0.67	0	2,2,2	0.33	0
2	EDO	A	501	-	3,3,3	0.68	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	B	501	-	3,3,3	0.53	0	2,2,2	0.69	0
2	EDO	C	502	-	3,3,3	0.65	0	2,2,2	0.21	0
2	EDO	C	501	-	3,3,3	0.55	0	2,2,2	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502	EDO	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	EDO	3	0
2	C	502	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.