Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:27 pm BST

PDB ID	:	6GDT
Title	:	Crystal structure of exo-glucosidase/glucosaminidase VC0615 from Vibrio Cholerae
Authors	:	Wu, L.; Davies, G.J.
Deposited on	:	2018-04-24
Resolution	:	3.17 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

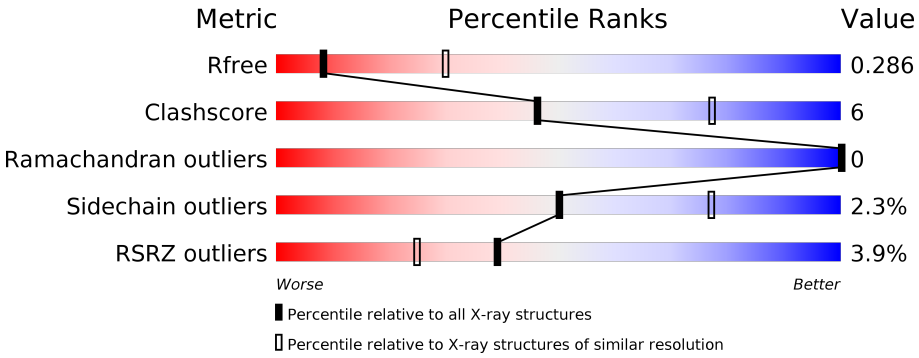
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	82% 15%
1	B	582	82% 15%
1	C	582	% 84% 13%
1	D	582	% 83% 14%
1	E	582	17% 78% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22709 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 Endoglucanase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4532	2871	793	844	24			
1	B	566	Total	C	N	O	S	0	0	0
			4532	2871	793	844	24			
1	C	566	Total	C	N	O	S	0	0	0
			4532	2871	793	844	24			
1	D	566	Total	C	N	O	S	0	0	0
			4532	2871	793	844	24			
1	E	562	Total	C	N	O	S	0	0	0
			4506	2857	789	836	24			

There are 40 discrepancies between the modelled and reference sequences:

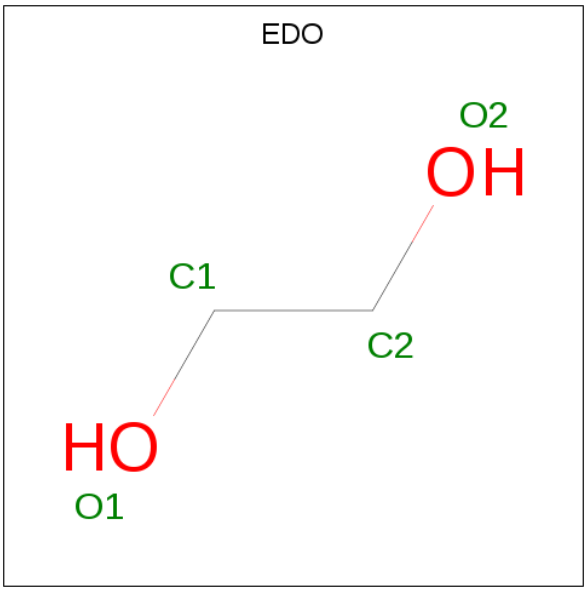
Chain	Residue	Modelled	Actual	Comment	Reference
A	575	LEU	-	expression tag	UNP Q9KUA8
A	576	GLU	-	expression tag	UNP Q9KUA8
A	577	HIS	-	expression tag	UNP Q9KUA8
A	578	HIS	-	expression tag	UNP Q9KUA8
A	579	HIS	-	expression tag	UNP Q9KUA8
A	580	HIS	-	expression tag	UNP Q9KUA8
A	581	HIS	-	expression tag	UNP Q9KUA8
A	582	HIS	-	expression tag	UNP Q9KUA8
B	575	LEU	-	expression tag	UNP Q9KUA8
B	576	GLU	-	expression tag	UNP Q9KUA8
B	577	HIS	-	expression tag	UNP Q9KUA8
B	578	HIS	-	expression tag	UNP Q9KUA8
B	579	HIS	-	expression tag	UNP Q9KUA8
B	580	HIS	-	expression tag	UNP Q9KUA8
B	581	HIS	-	expression tag	UNP Q9KUA8
B	582	HIS	-	expression tag	UNP Q9KUA8
C	575	LEU	-	expression tag	UNP Q9KUA8
C	576	GLU	-	expression tag	UNP Q9KUA8
C	577	HIS	-	expression tag	UNP Q9KUA8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	578	HIS	-	expression tag	UNP Q9KUA8
C	579	HIS	-	expression tag	UNP Q9KUA8
C	580	HIS	-	expression tag	UNP Q9KUA8
C	581	HIS	-	expression tag	UNP Q9KUA8
C	582	HIS	-	expression tag	UNP Q9KUA8
D	575	LEU	-	expression tag	UNP Q9KUA8
D	576	GLU	-	expression tag	UNP Q9KUA8
D	577	HIS	-	expression tag	UNP Q9KUA8
D	578	HIS	-	expression tag	UNP Q9KUA8
D	579	HIS	-	expression tag	UNP Q9KUA8
D	580	HIS	-	expression tag	UNP Q9KUA8
D	581	HIS	-	expression tag	UNP Q9KUA8
D	582	HIS	-	expression tag	UNP Q9KUA8
E	575	LEU	-	expression tag	UNP Q9KUA8
E	576	GLU	-	expression tag	UNP Q9KUA8
E	577	HIS	-	expression tag	UNP Q9KUA8
E	578	HIS	-	expression tag	UNP Q9KUA8
E	579	HIS	-	expression tag	UNP Q9KUA8
E	580	HIS	-	expression tag	UNP Q9KUA8
E	581	HIS	-	expression tag	UNP Q9KUA8
E	582	HIS	-	expression tag	UNP Q9KUA8

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



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

- Molecule 3 is water.

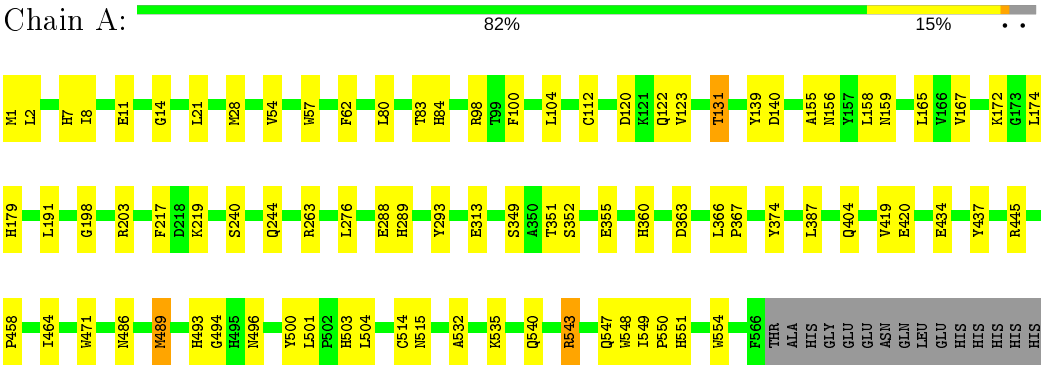
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	18	Total O 18 18	0	0
3	C	11	Total O 11 11	0	0
3	D	17	Total O 17 17	0	0
3	E	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

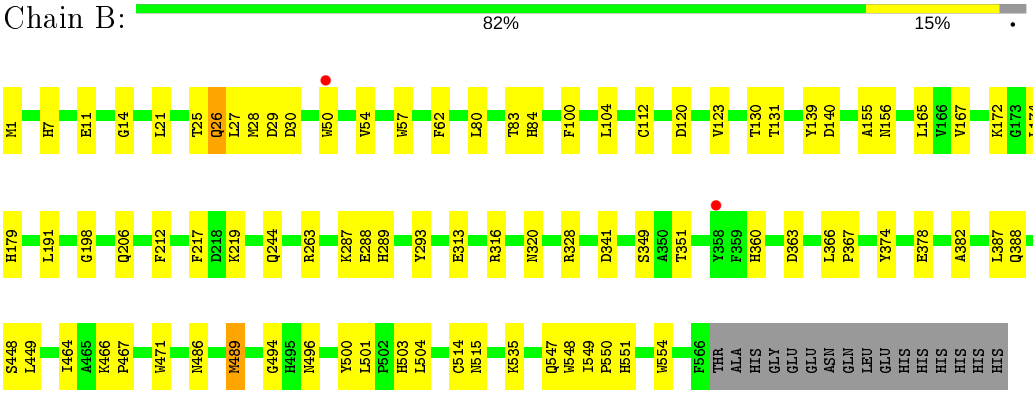
- Molecule 1: Endoglucanase-related protein

Chain A:



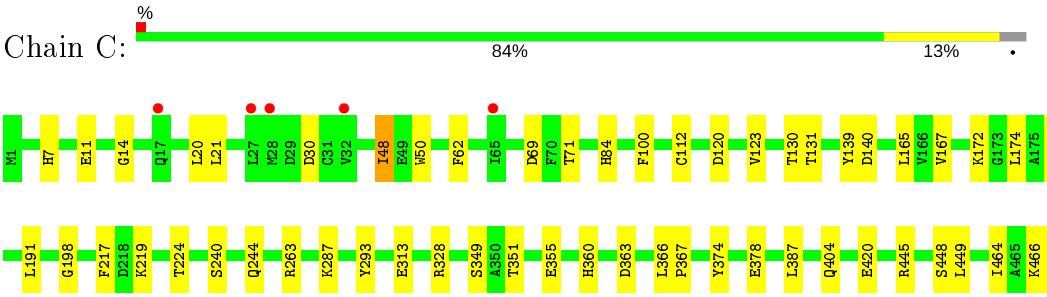
- Molecule 1: Endoglucanase-related protein

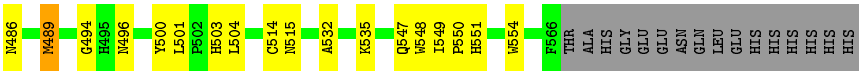
Chain B:



- Molecule 1: Endoglucanase-related protein

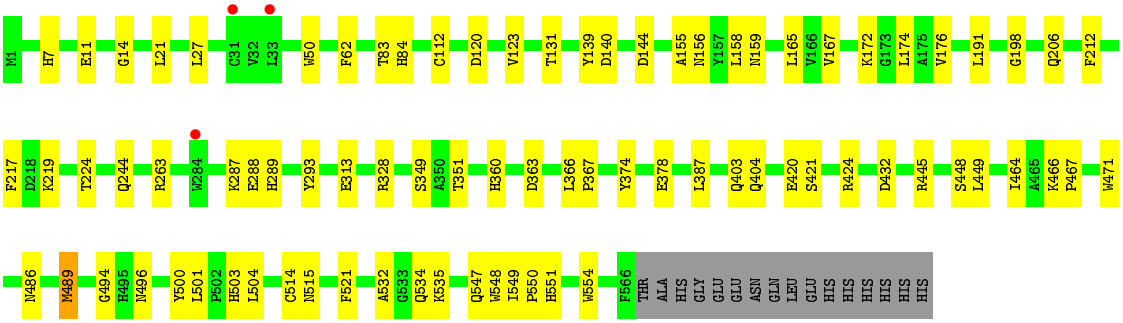
Chain C:





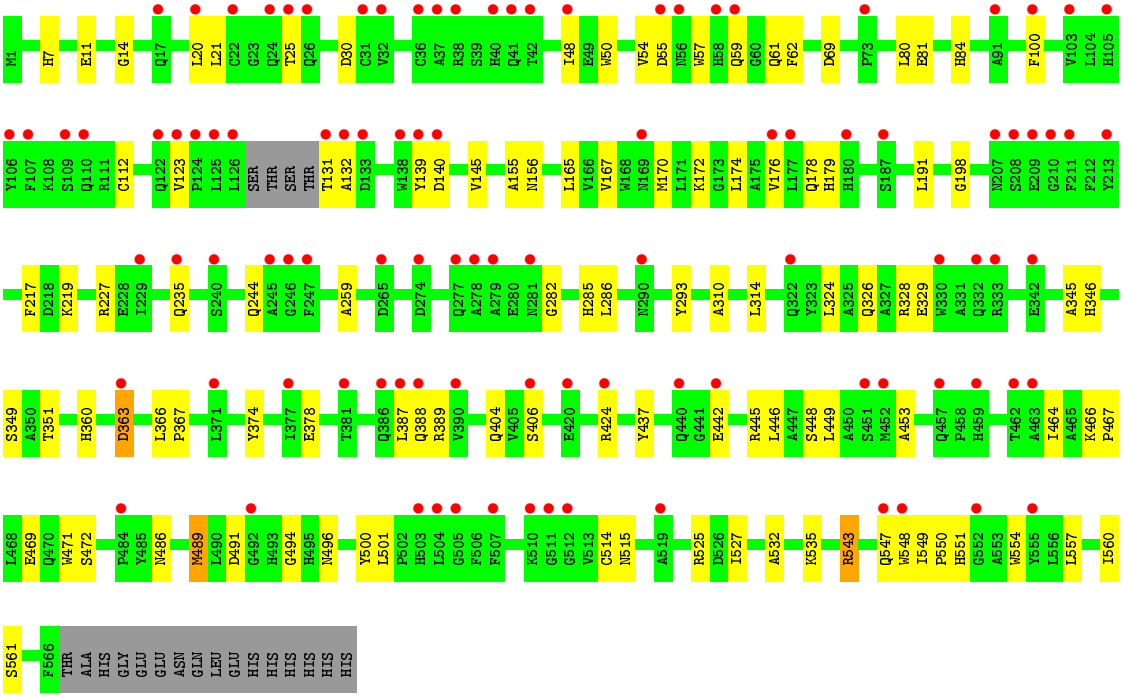
• Molecule 1: Endoglucanase-related protein

Chain D:



• Molecule 1: Endoglucanase-related protein

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	234.90Å 234.90Å 129.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 3.17 47.33 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.33-3.17) 99.9 (47.33-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.235 , 0.280 0.238 , 0.286	Depositor DCC
R_{free} test set	3411 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 20.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22709	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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

5.1 Standard geometry

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	0.42	0/4659	0.65	4/6330 (0.1%)
1	B	0.42	0/4659	0.65	0/6330
1	C	0.41	0/4659	0.63	0/6330
1	D	0.40	0/4659	0.64	0/6330
1	E	0.38	0/4632	0.63	1/6291 (0.0%)
All	All	0.41	0/23268	0.64	5/31611 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	543	ARG	CG-CD-NE	-8.54	93.86	111.80
1	A	543	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	98	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	203	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	131	THR	CA-CB-OG1	5.15	119.82	109.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4532	0	4269	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4532	0	4269	53	0
1	C	4532	0	4269	47	1
1	D	4532	0	4269	47	0
1	E	4506	0	4244	87	0
2	C	4	0	6	0	0
3	A	19	0	0	0	0
3	B	18	0	0	0	0
3	C	11	0	0	0	0
3	D	17	0	0	1	0
3	E	6	0	0	0	0
All	All	22709	0	21326	278	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 6.

All (278) 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:A:437:TYR:O	1:A:543:ARG:NH2	1.88	1.05
1:C:366:LEU:HD11	1:C:554:TRP:HZ2	1.25	0.99
1:C:366:LEU:HD11	1:C:554:TRP:CZ2	2.02	0.93
1:B:341:ASP:O	1:E:389:ARG:NH1	2.12	0.83
1:E:310:ALA:O	1:E:314:LEU:HD23	1.79	0.83
1:E:453:ALA:HB3	1:E:472:SER:OG	1.82	0.80
1:E:324:LEU:HD23	1:E:324:LEU:O	1.82	0.79
1:E:437:TYR:O	1:E:543:ARG:NH1	2.15	0.79
1:E:59:GLN:OE1	1:E:527:ILE:HD11	1.82	0.79
1:E:560:ILE:HD12	1:E:561:SER:N	1.98	0.78
1:C:366:LEU:CD1	1:C:554:TRP:HZ2	1.97	0.77
1:C:366:LEU:CD1	1:C:554:TRP:CZ2	2.68	0.77
1:B:26:GLN:HA	1:E:50:TRP:CG	2.20	0.76
1:A:263:ARG:NH1	1:A:313:GLU:OE1	2.19	0.76
1:B:25:THR:HG23	1:B:27:LEU:HD12	1.67	0.76
1:E:285:HIS:HE1	1:E:293:TYR:HE2	1.32	0.75
1:E:557:LEU:HD12	1:E:560:ILE:HD11	1.67	0.75
1:B:263:ARG:NH1	1:B:313:GLU:OE1	2.19	0.75
1:C:263:ARG:NH1	1:C:313:GLU:OE1	2.21	0.73
1:D:263:ARG:NH1	1:D:313:GLU:OE1	2.21	0.72
1:A:352:SER:OG	1:C:420:GLU:OE1	2.05	0.72
1:B:26:GLN:HA	1:E:50:TRP:CD2	2.26	0.71
1:A:240:SER:HB3	1:C:240:SER:HB3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLN:OE1	1:A:543:ARG:NH1	2.26	0.69
1:E:174:LEU:HG	1:E:191:LEU:HD13	1.72	0.69
1:D:421:SER:HB2	1:D:424:ARG:HH12	1.58	0.68
1:D:349:SER:OG	1:D:351:THR:O	2.13	0.67
1:C:363:ASP:HB3	1:C:366:LEU:HD13	1.75	0.66
1:C:349:SER:OG	1:C:351:THR:O	2.14	0.66
1:E:285:HIS:HE1	1:E:293:TYR:CE2	2.13	0.66
1:B:503:HIS:CE1	1:B:504:LEU:HD13	2.31	0.66
1:E:453:ALA:CB	1:E:472:SER:OG	2.44	0.65
1:D:503:HIS:CE1	1:D:504:LEU:HD13	2.32	0.65
1:E:349:SER:OG	1:E:351:THR:O	2.14	0.64
1:B:349:SER:OG	1:B:351:THR:O	2.13	0.63
1:C:48:ILE:HG21	1:C:50:TRP:CH2	2.32	0.63
1:E:360:HIS:CD2	1:E:363:ASP:OD1	2.52	0.63
1:E:326:GLN:O	1:E:329:GLU:HG2	1.99	0.63
1:B:1:MET:HE2	1:B:80:LEU:HD23	1.81	0.62
1:E:80:LEU:O	1:E:81:GLU:HG2	1.99	0.62
1:A:349:SER:OG	1:A:351:THR:O	2.15	0.62
1:A:122:GLN:HG2	1:A:131:THR:HG21	1.83	0.60
1:E:57:TRP:NE1	1:E:527:ILE:HG23	2.17	0.59
1:E:282:GLY:O	1:E:286:LEU:HD23	2.03	0.59
1:E:20:LEU:HD23	1:E:48:ILE:HD11	1.83	0.59
1:E:442:GLU:O	1:E:446:LEU:HD23	2.03	0.58
1:A:8:ILE:HD11	1:A:493:HIS:HB3	1.84	0.58
1:E:48:ILE:HG21	1:E:50:TRP:CH2	2.38	0.58
1:E:557:LEU:O	1:E:560:ILE:HG13	2.03	0.58
1:E:548:TRP:HB3	1:E:551:HIS:CD2	2.39	0.57
1:C:503:HIS:CD2	1:C:504:LEU:CD1	2.87	0.57
1:A:165:LEU:HD21	1:A:554:TRP:NE1	2.20	0.56
1:C:20:LEU:CD2	1:C:48:ILE:HD11	2.35	0.56
1:E:324:LEU:CD2	1:E:328:ARG:HG3	2.35	0.56
1:E:165:LEU:HD21	1:E:554:TRP:NE1	2.19	0.56
1:A:503:HIS:CE1	1:A:504:LEU:HD13	2.40	0.56
1:A:514:CYS:HA	1:A:547:GLN:HA	1.88	0.56
1:D:165:LEU:HD21	1:D:554:TRP:NE1	2.21	0.56
1:B:165:LEU:HD21	1:B:554:TRP:NE1	2.20	0.56
1:B:503:HIS:CE1	1:B:504:LEU:CD1	2.89	0.55
1:C:165:LEU:HD21	1:C:554:TRP:NE1	2.22	0.55
1:C:515:ASN:HA	1:C:551:HIS:NE2	2.21	0.55
1:E:449:LEU:HB3	1:E:471:TRP:CH2	2.42	0.55
1:A:515:ASN:HA	1:A:551:HIS:NE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LEU:HB3	1:B:471:TRP:CH2	2.42	0.55
1:B:50:TRP:CD1	1:E:406:SER:HB2	2.42	0.55
1:C:449:LEU:HB3	1:C:471:TRP:CH2	2.41	0.55
1:E:532:ALA:HA	1:E:535:LYS:HD2	1.89	0.55
1:E:57:TRP:CD1	1:E:527:ILE:HG23	2.42	0.55
1:E:360:HIS:NE2	1:E:363:ASP:OD1	2.41	0.54
1:A:449:LEU:HB3	1:A:471:TRP:CH2	2.42	0.54
1:D:503:HIS:CE1	1:D:504:LEU:CD1	2.90	0.54
1:D:449:LEU:HB3	1:D:471:TRP:CH2	2.41	0.54
1:C:514:CYS:HA	1:C:547:GLN:HA	1.89	0.54
1:E:145:VAL:O	1:E:227:ARG:NH1	2.41	0.54
1:D:515:ASN:HA	1:D:551:HIS:NE2	2.22	0.54
1:E:20:LEU:CD2	1:E:48:ILE:HD11	2.38	0.54
1:A:503:HIS:CE1	1:A:504:LEU:CD1	2.90	0.54
1:A:486:ASN:O	1:A:496:ASN:ND2	2.35	0.53
1:B:515:ASN:HA	1:B:551:HIS:NE2	2.23	0.53
1:D:514:CYS:HA	1:D:547:GLN:HA	1.89	0.53
1:B:514:CYS:HA	1:B:547:GLN:HA	1.91	0.53
1:B:363:ASP:HB3	1:B:366:LEU:HD12	1.90	0.53
1:B:486:ASN:O	1:B:496:ASN:ND2	2.36	0.52
1:D:363:ASP:HB3	1:D:366:LEU:HD12	1.91	0.52
1:E:514:CYS:HA	1:E:547:GLN:HA	1.90	0.52
1:D:206:GLN:HB2	1:D:212:PHE:CE1	2.45	0.52
1:B:206:GLN:HB2	1:B:212:PHE:CE1	2.45	0.52
1:B:503:HIS:ND1	1:B:504:LEU:CD1	2.73	0.51
1:E:80:LEU:C	1:E:81:GLU:HG2	2.30	0.51
1:A:244:GLN:HG2	1:A:293:TYR:CE1	2.46	0.51
1:E:324:LEU:HD22	1:E:328:ARG:NE	2.25	0.51
1:A:532:ALA:HA	1:A:535:LYS:HD2	1.92	0.51
1:D:420:GLU:HG2	1:D:432:ASP:OD2	2.10	0.51
1:A:548:TRP:HB3	1:A:551:HIS:CD2	2.46	0.51
1:C:21:LEU:HD13	1:C:62:PHE:CE1	2.46	0.50
1:C:20:LEU:HD23	1:C:48:ILE:HD11	1.93	0.50
1:C:486:ASN:O	1:C:496:ASN:ND2	2.37	0.50
1:A:363:ASP:HB3	1:A:366:LEU:HD12	1.93	0.50
1:A:503:HIS:ND1	1:A:504:LEU:CD1	2.74	0.50
1:C:112:CYS:HA	1:C:139:TYR:CE1	2.46	0.50
1:D:21:LEU:HD13	1:D:62:PHE:CE1	2.46	0.50
1:E:59:GLN:OE1	1:E:527:ILE:CD1	2.58	0.50
1:A:21:LEU:HD13	1:A:62:PHE:CE1	2.47	0.50
1:A:112:CYS:HA	1:A:139:TYR:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASP:HA	3:D:604:HOH:O	2.11	0.50
1:E:324:LEU:CD2	1:E:324:LEU:C	2.80	0.50
1:C:355:GLU:OE1	1:C:355:GLU:HA	2.11	0.50
1:B:54:VAL:HG21	1:B:57:TRP:CE3	2.46	0.50
1:B:112:CYS:HA	1:B:139:TYR:CE1	2.47	0.49
1:B:360:HIS:O	1:B:445:ARG:HD2	2.12	0.49
1:A:276:LEU:HD23	1:A:276:LEU:O	2.13	0.49
1:B:21:LEU:HD13	1:B:62:PHE:CE1	2.46	0.49
1:D:244:GLN:HG2	1:D:293:TYR:CE1	2.48	0.49
1:B:172:LYS:O	1:B:176:VAL:HG23	2.12	0.49
1:E:244:GLN:HG2	1:E:293:TYR:CE1	2.47	0.49
1:E:324:LEU:HD23	1:E:324:LEU:C	2.32	0.49
1:E:360:HIS:O	1:E:445:ARG:HD2	2.13	0.49
1:A:360:HIS:O	1:A:445:ARG:HD2	2.12	0.49
1:D:503:HIS:ND1	1:D:504:LEU:CD1	2.76	0.49
1:D:360:HIS:O	1:D:445:ARG:HD2	2.13	0.49
1:E:25:THR:HG22	1:E:61:GLN:HE21	1.78	0.49
1:A:28:MET:SD	1:A:28:MET:N	2.86	0.49
1:C:244:GLN:HG2	1:C:293:TYR:CE1	2.48	0.49
1:C:360:HIS:O	1:C:445:ARG:HD2	2.13	0.49
1:D:421:SER:HB2	1:D:424:ARG:NH1	2.28	0.49
1:D:548:TRP:HB3	1:D:551:HIS:CD2	2.48	0.49
1:C:548:TRP:HB3	1:C:551:HIS:CD2	2.48	0.48
1:E:57:TRP:CG	1:E:527:ILE:HG12	2.48	0.48
1:D:112:CYS:HA	1:D:139:TYR:CE1	2.48	0.48
1:D:374:TYR:CE2	1:D:387:LEU:HD13	2.48	0.48
1:E:112:CYS:HA	1:E:139:TYR:CE1	2.48	0.48
1:E:363:ASP:HB2	1:E:366:LEU:HD12	1.96	0.48
1:E:11:GLU:HB2	1:E:14:GLY:HA3	1.96	0.48
1:A:374:TYR:CE2	1:A:387:LEU:HD13	2.49	0.48
1:B:549:ILE:N	1:B:550:PRO:CD	2.76	0.48
1:E:548:TRP:HB3	1:E:551:HIS:NE2	2.29	0.48
1:A:172:LYS:O	1:A:176:VAL:HG13	2.14	0.47
1:E:324:LEU:HD23	1:E:328:ARG:HG3	1.96	0.47
1:A:549:ILE:N	1:A:550:PRO:CD	2.77	0.47
1:E:374:TYR:CE2	1:E:387:LEU:HD13	2.49	0.47
1:E:55:ASP:OD1	1:E:525:ARG:CZ	2.62	0.47
1:D:549:ILE:N	1:D:550:PRO:CD	2.77	0.47
1:C:172:LYS:O	1:C:176:VAL:HG13	2.14	0.47
1:D:532:ALA:HA	1:D:535:LYS:HD2	1.95	0.47
1:E:123:VAL:HG12	1:E:132:ALA:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:ILE:N	1:E:550:PRO:CD	2.77	0.47
1:B:244:GLN:HG2	1:B:293:TYR:CE1	2.48	0.47
1:B:548:TRP:HB3	1:B:551:HIS:CD2	2.49	0.47
1:D:172:LYS:O	1:D:176:VAL:HG13	2.13	0.47
1:E:442:GLU:O	1:E:446:LEU:CD2	2.63	0.47
1:A:1:MET:CE	1:A:80:LEU:HD12	2.45	0.47
1:E:324:LEU:CD2	1:E:324:LEU:O	2.59	0.47
1:C:549:ILE:N	1:C:550:PRO:CD	2.78	0.46
1:B:288:GLU:OE2	1:B:289:HIS:NE2	2.48	0.46
1:D:11:GLU:HB2	1:D:14:GLY:HA3	1.98	0.46
1:D:7:HIS:HB3	1:D:494:GLY:HA2	1.98	0.46
1:E:172:LYS:O	1:E:176:VAL:HG13	2.15	0.46
1:E:174:LEU:HD21	1:E:191:LEU:HB3	1.97	0.46
1:A:288:GLU:OE2	1:A:289:HIS:NE2	2.49	0.46
1:E:259:ALA:CB	1:E:314:LEU:HD22	2.45	0.46
1:B:11:GLU:HB2	1:B:14:GLY:HA3	1.97	0.46
1:E:560:ILE:HD12	1:E:560:ILE:C	2.37	0.46
1:C:374:TYR:CE2	1:C:387:LEU:HD13	2.51	0.46
1:B:374:TYR:CE2	1:B:387:LEU:HD13	2.51	0.45
1:C:11:GLU:HB2	1:C:14:GLY:HA3	1.97	0.45
1:E:21:LEU:HD13	1:E:62:PHE:CE1	2.51	0.45
1:D:288:GLU:OE2	1:D:289:HIS:NE2	2.48	0.45
1:D:486:ASN:O	1:D:496:ASN:ND2	2.37	0.45
1:E:466:LYS:HA	1:E:469:GLU:OE1	2.17	0.45
1:A:54:VAL:HG11	1:A:57:TRP:CE3	2.52	0.45
1:E:54:VAL:HG11	1:E:57:TRP:CE3	2.51	0.45
1:C:7:HIS:HB3	1:C:494:GLY:HA2	1.99	0.45
1:B:489:MET:CG	1:B:514:CYS:SG	3.05	0.45
1:E:170:MET:HB3	1:E:191:LEU:HD21	1.99	0.44
1:E:486:ASN:O	1:E:496:ASN:ND2	2.37	0.44
1:A:489:MET:CG	1:A:514:CYS:SG	3.05	0.44
1:D:448:SER:HA	1:D:554:TRP:CE3	2.52	0.44
1:E:515:ASN:HA	1:E:551:HIS:CE1	2.53	0.44
1:E:7:HIS:HB3	1:E:494:GLY:HA2	2.00	0.44
1:B:26:GLN:HG3	1:B:28:MET:CE	2.48	0.44
1:B:7:HIS:HB3	1:B:494:GLY:HA2	2.00	0.44
1:D:167:VAL:HG22	1:D:198:GLY:HA3	2.00	0.44
1:D:489:MET:CG	1:D:514:CYS:SG	3.05	0.44
1:C:448:SER:HA	1:C:554:TRP:CE3	2.53	0.44
1:C:489:MET:CG	1:C:514:CYS:SG	3.05	0.44
1:B:26:GLN:HG3	1:B:28:MET:HE3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:SER:HA	1:B:554:TRP:CE3	2.52	0.44
1:C:20:LEU:HD22	1:C:48:ILE:HD11	2.00	0.44
1:D:366:LEU:O	1:D:367:PRO:C	2.56	0.44
1:B:26:GLN:H	1:B:26:GLN:HG2	1.57	0.44
1:E:448:SER:HA	1:E:554:TRP:CE3	2.53	0.44
1:A:464:ILE:O	1:A:464:ILE:HG23	2.17	0.43
1:B:167:VAL:HG22	1:B:198:GLY:HA3	1.99	0.43
1:E:366:LEU:O	1:E:367:PRO:C	2.57	0.43
1:E:489:MET:CG	1:E:514:CYS:SG	3.06	0.43
1:A:165:LEU:HD21	1:A:554:TRP:CD1	2.54	0.43
1:B:489:MET:HG2	1:B:514:CYS:SG	2.59	0.43
1:B:366:LEU:O	1:B:367:PRO:C	2.57	0.43
1:A:217:PHE:CE2	1:A:219:LYS:HA	2.54	0.43
1:C:167:VAL:HG22	1:C:198:GLY:HA3	2.00	0.43
1:E:57:TRP:CE2	1:E:527:ILE:HG21	2.54	0.43
1:A:500:TYR:CE2	1:A:501:LEU:HD12	2.54	0.43
1:D:420:GLU:HG3	1:D:420:GLU:O	2.19	0.43
1:E:191:LEU:HD23	1:E:191:LEU:O	2.19	0.43
1:C:489:MET:HG2	1:C:514:CYS:SG	2.58	0.43
1:A:174:LEU:HD21	1:A:191:LEU:HB3	2.01	0.43
1:A:448:SER:HA	1:A:554:TRP:CE3	2.53	0.43
1:B:174:LEU:HD21	1:B:191:LEU:HB3	2.01	0.43
1:A:489:MET:HG2	1:A:514:CYS:SG	2.59	0.42
1:E:170:MET:HB3	1:E:191:LEU:CD2	2.49	0.42
1:C:178:GLN:O	1:C:179:HIS:HB2	2.20	0.42
1:E:217:PHE:CE2	1:E:219:LYS:HA	2.55	0.42
1:A:120:ASP:HA	1:A:123:VAL:CG2	2.50	0.42
1:B:217:PHE:CE2	1:B:219:LYS:HA	2.55	0.42
1:B:26:GLN:O	1:B:27:LEU:HB2	2.20	0.42
1:A:11:GLU:HB2	1:A:14:GLY:HA3	2.01	0.42
1:A:7:HIS:HB3	1:A:494:GLY:HA2	2.01	0.42
1:B:500:TYR:CE2	1:B:501:LEU:HD12	2.55	0.42
1:D:464:ILE:O	1:D:464:ILE:HG23	2.18	0.42
1:D:521:PHE:CE2	1:D:534:GLN:HG2	2.54	0.42
1:E:345:ALA:HB1	1:E:346:HIS:CD2	2.55	0.42
1:A:1:MET:HE3	1:A:80:LEU:HD12	2.01	0.42
1:B:165:LEU:HD21	1:B:554:TRP:CD1	2.55	0.42
1:C:500:TYR:CE2	1:C:501:LEU:HD12	2.54	0.42
1:D:500:TYR:CE2	1:D:501:LEU:HD12	2.55	0.42
1:D:489:MET:HG2	1:D:514:CYS:SG	2.60	0.42
1:E:167:VAL:HG22	1:E:198:GLY:HA3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HD13	1:D:50:TRP:CZ3	2.54	0.42
1:E:57:TRP:CE2	1:E:527:ILE:CG2	3.02	0.42
1:B:178:GLN:O	1:B:179:HIS:HB2	2.20	0.42
1:D:217:PHE:CE2	1:D:219:LYS:HA	2.55	0.42
1:E:165:LEU:HD21	1:E:554:TRP:CD1	2.55	0.42
1:A:366:LEU:O	1:A:367:PRO:C	2.56	0.42
1:D:155:ALA:O	1:D:156:ASN:HB2	2.20	0.42
1:D:165:LEU:HD21	1:D:554:TRP:CD1	2.55	0.42
1:E:500:TYR:CE2	1:E:501:LEU:HD12	2.55	0.41
1:A:155:ALA:O	1:A:156:ASN:HB2	2.20	0.41
1:B:155:ALA:O	1:B:156:ASN:HB2	2.20	0.41
1:C:464:ILE:HG23	1:C:464:ILE:O	2.20	0.41
1:A:167:VAL:HG22	1:A:198:GLY:HA3	2.02	0.41
1:B:26:GLN:HB3	1:E:50:TRP:CE3	2.55	0.41
1:E:464:ILE:HG23	1:E:464:ILE:O	2.20	0.41
1:C:217:PHE:CE2	1:C:219:LYS:HA	2.54	0.41
1:A:420:GLU:HG2	1:C:351:THR:HB	2.01	0.41
1:C:366:LEU:O	1:C:367:PRO:C	2.57	0.41
1:A:178:GLN:O	1:A:179:HIS:HB2	2.19	0.41
1:B:328:ARG:NH1	1:B:378:GLU:OE1	2.53	0.41
1:C:174:LEU:HD21	1:C:191:LEU:HB3	2.02	0.41
1:C:328:ARG:NH1	1:C:378:GLU:OE1	2.53	0.41
1:D:328:ARG:NH1	1:D:378:GLU:OE1	2.53	0.41
1:E:489:MET:HG2	1:E:514:CYS:SG	2.61	0.41
1:C:165:LEU:HD21	1:C:554:TRP:CD1	2.55	0.41
1:D:174:LEU:HD21	1:D:191:LEU:HB3	2.02	0.41
1:E:328:ARG:NH1	1:E:378:GLU:OE1	2.54	0.41
1:B:464:ILE:O	1:B:464:ILE:HG23	2.21	0.41
1:C:120:ASP:HA	1:C:123:VAL:CG2	2.51	0.41
1:C:532:ALA:HA	1:C:535:LYS:HD2	2.03	0.41
1:D:466:LYS:N	1:D:467:PRO:CD	2.84	0.41
1:E:178:GLN:O	1:E:179:HIS:HB2	2.21	0.41
1:D:120:ASP:HA	1:D:123:VAL:CG2	2.51	0.41
1:B:104:LEU:HA	1:B:104:LEU:HD12	1.92	0.41
1:B:120:ASP:HA	1:B:123:VAL:CG2	2.51	0.41
1:A:100:PHE:CD1	1:A:100:PHE:C	2.94	0.40
1:A:419:VAL:HG12	1:A:434:GLU:HG3	2.02	0.40
1:B:466:LYS:N	1:B:467:PRO:CD	2.84	0.40
1:C:100:PHE:C	1:C:100:PHE:CD1	2.94	0.40
1:C:466:LYS:N	1:C:467:PRO:CD	2.84	0.40
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLN:N	1:A:458:PRO:HD2	2.37	0.40
1:E:100:PHE:C	1:E:100:PHE:CD1	2.95	0.40
1:E:174:LEU:CG	1:E:191:LEU:HD13	2.46	0.40
1:A:158:LEU:O	1:A:159:ASN:C	2.59	0.40
1:B:382:ALA:HB3	1:D:424:ARG:NH2	2.36	0.40
1:E:155:ALA:O	1:E:156:ASN:HB2	2.21	0.40
1:B:100:PHE:C	1:B:100:PHE:CD1	2.94	0.40
1:D:158:LEU:O	1:D:159:ASN:C	2.59	0.40
1:E:466:LYS:HB2	1:E:467:PRO:HD3	2.02	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:C:69:ASP:O	1:C:71:THR:OG1[5_555]	2.06	0.14

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	564/582 (97%)	528 (94%)	36 (6%)	0	100	100
1	B	564/582 (97%)	528 (94%)	36 (6%)	0	100	100
1	C	564/582 (97%)	529 (94%)	35 (6%)	0	100	100
1	D	564/582 (97%)	528 (94%)	36 (6%)	0	100	100
1	E	558/582 (96%)	524 (94%)	34 (6%)	0	100	100
All	All	2814/2910 (97%)	2637 (94%)	177 (6%)	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	467/481 (97%)	460 (98%)	7 (2%)	65	85
1	B	467/481 (97%)	452 (97%)	15 (3%)	39	70
1	C	467/481 (97%)	457 (98%)	10 (2%)	53	79
1	D	467/481 (97%)	458 (98%)	9 (2%)	57	80
1	E	463/481 (96%)	451 (97%)	12 (3%)	46	75
All	All	2331/2405 (97%)	2278 (98%)	53 (2%)	50	77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	84	HIS
1	A	104	LEU
1	A	140	ASP
1	A	355	GLU
1	A	404	GLN
1	A	489	MET
1	B	26	GLN
1	B	29	ASP
1	B	30	ASP
1	B	83	THR
1	B	84	HIS
1	B	130	THR
1	B	131	THR
1	B	140	ASP
1	B	287	LYS
1	B	316	ARG
1	B	320	ASN
1	B	388	GLN
1	B	404	GLN
1	B	489	MET
1	B	535	LYS
1	C	30	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	48	ILE
1	C	84	HIS
1	C	130	THR
1	C	131	THR
1	C	140	ASP
1	C	224	THR
1	C	287	LYS
1	C	404	GLN
1	C	489	MET
1	D	83	THR
1	D	84	HIS
1	D	131	THR
1	D	140	ASP
1	D	224	THR
1	D	287	LYS
1	D	403	GLN
1	D	404	GLN
1	D	489	MET
1	E	30	ASP
1	E	69	ASP
1	E	84	HIS
1	E	131	THR
1	E	140	ASP
1	E	235	GLN
1	E	363	ASP
1	E	388	GLN
1	E	404	GLN
1	E	424	ARG
1	E	489	MET
1	E	491	ASP

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	C	601	-	3,3,3	0.63	0	2,2,2	0.08	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	C	601	-	-	0/1/1/1	-

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	566/582 (97%)	-0.49	0 100 100	60, 86, 111, 159	0
1	B	566/582 (97%)	-0.45	2 (0%) 92 89	61, 85, 110, 194	0
1	C	566/582 (97%)	-0.45	5 (0%) 84 75	63, 85, 110, 142	0
1	D	566/582 (97%)	-0.35	3 (0%) 91 86	67, 95, 118, 151	0
1	E	562/582 (96%)	0.95	101 (17%) 1 1	111, 174, 228, 297	0
All	All	2826/2910 (97%)	-0.16	111 (3%) 39 25	60, 91, 194, 297	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	278	ALA	6.9
1	E	109	SER	5.8
1	E	503	HIS	5.6
1	E	131	THR	5.5
1	E	246	GLY	5.3
1	E	388	GLN	5.3
1	E	387	LEU	5.2
1	E	210	GLY	5.1
1	E	59	GLN	5.0
1	E	209	GLU	4.9
1	E	462	THR	4.8
1	E	24	GLN	4.6
1	E	290	ASN	4.6
1	E	504	LEU	4.5
1	E	386	GLN	4.5
1	E	507	PHE	4.4
1	E	277	GLN	4.4
1	E	126	LEU	4.3
1	E	106	TYR	4.2
1	E	552	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	133	ASP	4.2
1	E	123	VAL	4.1
1	E	40	HIS	4.0
1	E	140	ASP	3.9
1	E	245	ALA	3.8
1	E	511	GLY	3.7
1	E	547	GLN	3.6
1	E	211	PHE	3.6
1	E	169	ASN	3.6
1	E	207	ASN	3.6
1	E	342	GLU	3.5
1	E	32	VAL	3.5
1	E	110	GLN	3.4
1	E	48	ILE	3.4
1	E	463	ALA	3.4
1	E	100	PHE	3.3
1	E	139	TYR	3.3
1	E	208	SER	3.3
1	E	279	ALA	3.3
1	E	381	THR	3.3
1	E	213	TYR	3.2
1	E	124	PRO	3.2
1	E	38	ARG	3.1
1	E	42	THR	3.1
1	E	274	ASP	3.1
1	E	363	ASP	3.1
1	E	371	LEU	3.1
1	E	22	CYS	3.1
1	E	125	LEU	3.1
1	E	247	PHE	3.0
1	E	322	GLN	3.0
1	E	330	TRP	2.9
1	E	505	GLY	2.9
1	E	177	LEU	2.9
1	D	31	CYS	2.9
1	E	512	GLY	2.9
1	E	103	VAL	2.9
1	E	333	ARG	2.8
1	E	281	ASN	2.8
1	D	284	TRP	2.8
1	E	510	LYS	2.8
1	E	176	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	492	GLY	2.8
1	E	37	ALA	2.7
1	E	122	GLN	2.7
1	E	451	SER	2.7
1	E	484	PRO	2.6
1	E	377	ILE	2.6
1	D	33	LEU	2.6
1	E	457	GLN	2.5
1	C	65	ILE	2.5
1	E	265	ASP	2.5
1	E	105	HIS	2.5
1	E	132	ALA	2.5
1	E	235	GLN	2.5
1	E	229	ILE	2.5
1	E	91	ALA	2.4
1	E	26	GLN	2.4
1	E	442	GLU	2.4
1	E	187	SER	2.4
1	E	420	GLU	2.4
1	C	17	GLN	2.4
1	E	440	GLN	2.3
1	E	73	PRO	2.3
1	E	107	PHE	2.3
1	E	56	ASN	2.3
1	E	519	ALA	2.3
1	C	32	VAL	2.3
1	E	390	VAL	2.3
1	E	406	SER	2.3
1	E	452	MET	2.3
1	C	27	LEU	2.2
1	E	180	HIS	2.2
1	E	240	SER	2.2
1	E	424	ARG	2.2
1	E	41	GLN	2.2
1	E	55	ASP	2.2
1	E	332	GLN	2.2
1	E	20	LEU	2.2
1	E	138	TRP	2.2
1	B	50	TRP	2.1
1	E	25	THR	2.1
1	E	17	GLN	2.1
1	C	28	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	58	HIS	2.1
1	E	459	HIS	2.1
1	E	548	TRP	2.0
1	B	358	TYR	2.0
1	E	31	CYS	2.0
1	E	36	CYS	2.0
1	E	555	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	601	4/4	0.95	0.40	68,76,80,81	0

6.5 Other polymers (i)

There are no such residues in this entry.