



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:39 PM UTC

PDB ID : 2VSY / pdb_00002vsy
Title : Xanthomonas campestris putative OGT (XCC0866), apostructure
Authors : Schuettelkopf, A.W.; Clarke, A.J.; van Aalten, D.M.F.
Deposited on : 2008-05-01
Resolution : 2.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

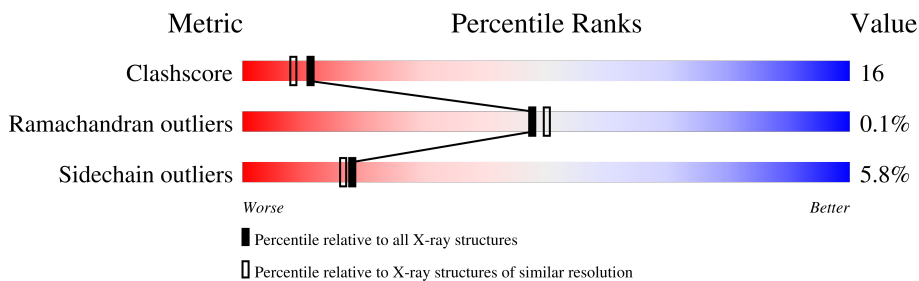
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	568	 73% 19% . .
1	B	568	 72% 21% . .

2 Entry composition [i](#)

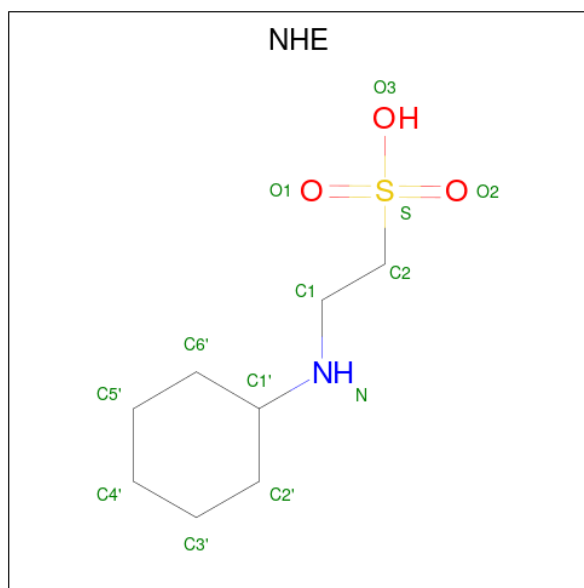
There are 6 unique types of molecules in this entry. The entry contains 8733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XCC0866.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	1	0
			4166	2632	770	748	16			
1	B	547	Total	C	N	O	S	0	4	0
			4189	2648	778	747	16			

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PRASEODYMIUM ION (CCD ID: PR) (formula: Pr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Pr	0	0
			2	2		
4	B	1	Total	Pr	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

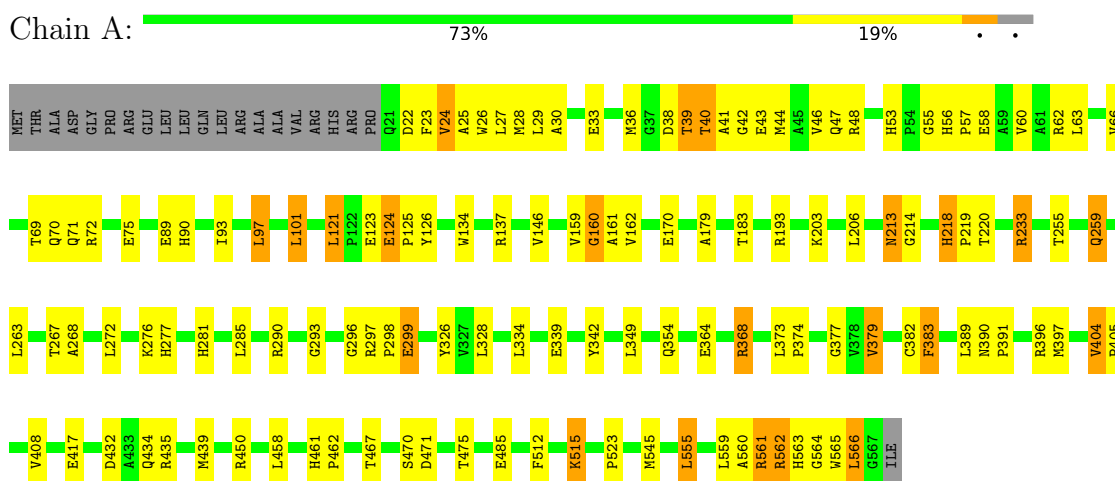
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	153	Total	O	0	0
			153	153		
6	B	167	Total	O	0	0
			167	167		

3 Residue-property plots

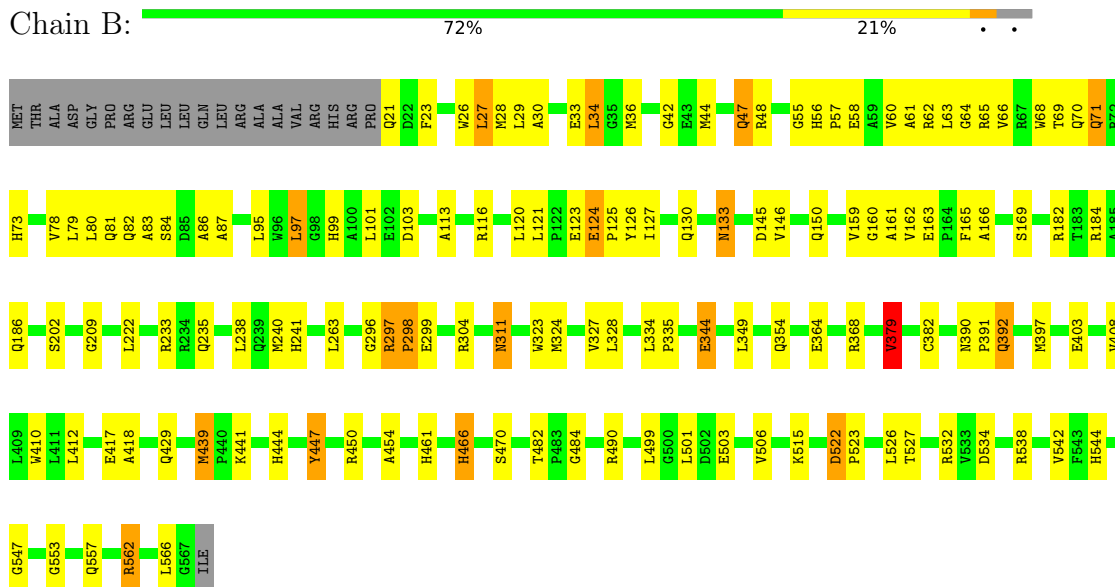
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: XCC0866



- Molecule 1: XCC0866



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.52Å 100.10Å 156.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.4 (20.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.193 , 0.236	Depositor
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.819	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8733	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PR, CL, NHE

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	0.90	1/4278 (0.0%)	1.08	18/5839 (0.3%)
1	B	0.96	1/4311 (0.0%)	1.10	17/5882 (0.3%)
All	All	0.93	2/8589 (0.0%)	1.09	35/11721 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	VAL	CA-CB	6.92	1.62	1.53
1	B	379	VAL	CA-CB	5.37	1.60	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	522	ASP	CA-C-N	10.61	131.42	119.32
1	B	522	ASP	C-N-CA	10.61	131.42	119.32
1	A	561	ARG	N-CA-C	-9.59	100.68	111.71
1	A	404	VAL	CA-C-N	7.13	128.76	119.84
1	A	404	VAL	C-N-CA	7.13	128.76	119.84
1	B	36	MET	N-CA-C	-7.02	104.75	113.38
1	B	161	ALA	N-CA-C	6.71	118.28	110.97
1	A	124	GLU	CA-C-N	6.62	126.20	119.19
1	A	124	GLU	C-N-CA	6.62	126.20	119.19
1	A	218	HIS	CA-C-N	6.52	126.02	119.24
1	A	218	HIS	C-N-CA	6.52	126.02	119.24
1	B	297	ARG	CA-C-N	6.38	127.81	119.84
1	B	297	ARG	C-N-CA	6.38	127.81	119.84
1	B	335	PRO	CA-C-N	6.35	126.56	119.32
1	B	335	PRO	C-N-CA	6.35	126.56	119.32
1	A	383	PHE	N-CA-C	-6.10	99.26	108.96
1	A	364	GLU	CA-C-N	-5.86	114.35	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	GLU	C-N-CA	-5.86	114.35	120.38
1	B	379	VAL	N-CA-C	5.80	115.96	107.37
1	B	364	GLU	CA-C-N	-5.63	114.58	120.38
1	B	364	GLU	C-N-CA	-5.63	114.58	120.38
1	B	235	GLN	CA-C-N	5.37	125.19	119.28
1	B	235	GLN	C-N-CA	5.37	125.19	119.28
1	B	439	MET	CA-C-N	-5.36	113.14	119.84
1	B	439	MET	C-N-CA	-5.36	113.14	119.84
1	A	562	ARG	CA-C-N	-5.34	114.09	122.79
1	A	562	ARG	C-N-CA	-5.34	114.09	122.79
1	A	160	GLY	N-CA-C	-5.25	107.79	115.72
1	B	124	GLU	CA-C-N	5.22	124.72	119.19
1	B	124	GLU	C-N-CA	5.22	124.72	119.19
1	A	170	GLU	CA-C-N	-5.18	114.79	122.41
1	A	170	GLU	C-N-CA	-5.18	114.79	122.41
1	A	146	VAL	N-CA-C	5.07	115.29	110.42
1	A	339	GLU	CA-C-N	-5.01	114.45	119.56
1	A	339	GLU	C-N-CA	-5.01	114.45	119.56

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	4166	0	4089	137	0
1	B	4189	0	4124	134	0
2	A	13	0	17	1	0
2	B	26	0	34	0	0
3	A	14	0	20	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	B	2	0	0	0	0
6	A	153	0	0	3	0
6	B	167	0	0	5	0
All	All	8733	0	8284	272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (272) 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:555:LEU:HD23	1:A:555:LEU:C	1.68	1.18
1:B:97:LEU:C	1:B:97:LEU:HD23	1.65	1.17
1:B:34:LEU:N	1:B:34:LEU:HD23	1.55	1.16
1:B:78:VAL:O	1:B:82:GLN:HG3	1.47	1.15
1:B:562:ARG:HH11	1:B:562:ARG:CG	1.63	1.10
1:B:562:ARG:HH11	1:B:562:ARG:HG2	1.16	1.08
1:B:97:LEU:HD23	1:B:97:LEU:O	1.54	1.08
1:B:499:LEU:HD23	1:B:501:LEU:HD12	1.30	1.08
1:A:97:LEU:CD2	1:A:101:LEU:HD22	1.84	1.07
1:B:30:ALA:O	1:B:34:LEU:HG	1.53	1.06
1:A:97:LEU:HD22	1:A:101:LEU:CD2	1.84	1.06
1:A:562:ARG:O	1:A:562:ARG:HD3	1.54	1.04
1:A:42:GLY:O	1:A:46:VAL:HG23	1.58	1.03
1:A:97:LEU:HD22	1:A:101:LEU:HD22	1.05	1.03
1:B:97:LEU:HD21	1:B:101:LEU:HD12	1.39	1.01
1:B:97:LEU:HD21	1:B:101:LEU:CD1	1.92	0.98
1:B:439:MET:HE1	1:B:447:TYR:HD1	1.25	0.97
1:A:555:LEU:HD23	1:A:555:LEU:O	1.61	0.97
1:A:63:LEU:HD12	1:A:63:LEU:O	1.63	0.97
1:B:97:LEU:C	1:B:97:LEU:CD2	2.37	0.96
1:A:90:HIS:CG	1:A:93:ILE:HD12	2.00	0.95
1:B:97:LEU:CD2	1:B:101:LEU:HD12	1.99	0.92
1:A:397:MET:HE2	1:A:458:LEU:HB2	1.53	0.90
1:B:34:LEU:N	1:B:34:LEU:CD2	2.32	0.90
1:A:159:VAL:HG23	1:A:161:ALA:H	1.37	0.89
1:A:43:GLU:O	1:A:47:GLN:HG2	1.74	0.88
1:B:499:LEU:HD13	1:B:542[A]:VAL:HG11	1.57	0.87
1:A:555:LEU:C	1:A:555:LEU:CD2	2.47	0.87
1:B:34:LEU:HD22	1:B:42:GLY:HA3	1.58	0.86
1:A:39:THR:OG1	1:A:40:THR:HG22	1.77	0.85
1:A:213:ASN:H	1:A:213:ASN:HD22	1.26	0.84
1:B:34:LEU:CD2	1:B:42:GLY:HA3	2.06	0.84
1:B:562:ARG:HG2	1:B:562:ARG:NH1	1.81	0.84
1:A:27:LEU:O	1:A:30:ALA:HB3	1.78	0.84
1:B:56:HIS:HD2	1:B:58:GLU:H	1.23	0.82
1:A:27:LEU:HB3	1:A:62:ARG:HD3	1.61	0.82
1:A:564:GLY:O	1:A:566:LEU:CD2	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:TRP:C	1:A:566:LEU:HD22	2.04	0.82
1:A:565:TRP:O	1:A:566:LEU:HD22	1.80	0.81
1:A:562:ARG:HD3	1:A:562:ARG:C	2.06	0.79
1:A:218:HIS:CG	1:A:219:PRO:HD2	2.18	0.79
1:B:439:MET:HE3	6:B:2129:HOH:O	1.82	0.79
1:B:33:GLU:C	1:B:34:LEU:HD23	2.08	0.78
1:B:120:LEU:O	1:B:121:LEU:HD23	1.83	0.78
1:B:124:GLU:HG3	1:B:127:ILE:HG12	1.65	0.78
1:A:564:GLY:O	1:A:566:LEU:HD23	1.83	0.78
1:B:499:LEU:HD23	1:B:501:LEU:CD1	2.11	0.77
1:A:27:LEU:O	1:A:30:ALA:N	2.19	0.76
1:A:383:PHE:CZ	1:A:439:MET:HE3	2.21	0.75
1:A:562:ARG:HD2	1:A:563:HIS:CD2	2.21	0.75
1:B:34:LEU:HD21	1:B:42:GLY:CA	2.15	0.75
1:B:439:MET:HE1	1:B:447:TYR:CD1	2.16	0.75
1:B:412:LEU:HD12	1:B:439:MET:HE2	1.69	0.74
1:A:461:HIS:HD2	6:A:2131:HOH:O	1.69	0.74
1:B:33:GLU:HB3	1:B:34:LEU:HD23	1.69	0.74
1:B:544[B]:HIS:HD2	1:B:547:GLY:H	1.35	0.73
1:B:34:LEU:HD23	1:B:34:LEU:H	1.51	0.73
1:A:397:MET:CE	1:A:458:LEU:HB2	2.19	0.72
1:A:29:LEU:HG	1:A:33:GLU:OE1	1.89	0.72
1:A:334:LEU:HD11	1:A:342:TYR:CE2	2.25	0.72
1:A:124:GLU:OE2	1:A:126:TYR:HB3	1.90	0.72
1:B:379:VAL:HG22	1:B:454:ALA:HA	1.70	0.72
1:A:562:ARG:O	1:A:562:ARG:CD	2.35	0.71
1:A:382:CYS:HB2	1:A:397:MET:HE1	1.72	0.71
1:B:34:LEU:HD21	1:B:42:GLY:HA2	1.71	0.71
1:B:73:HIS:ND1	1:B:103:ASP:HB3	2.05	0.71
1:B:544[B]:HIS:CD2	1:B:547:GLY:H	2.08	0.71
1:B:412:LEU:CD1	1:B:439:MET:HE2	2.20	0.71
1:A:218:HIS:CD2	1:A:220:THR:H	2.09	0.70
1:A:277:HIS:CE1	1:A:281:HIS:HE1	2.09	0.70
1:A:193:ARG:H	1:A:193:ARG:HD2	1.55	0.70
1:B:562:ARG:HH11	1:B:562:ARG:HG3	1.57	0.70
1:A:63:LEU:O	1:A:63:LEU:CD1	2.40	0.70
1:B:34:LEU:CD2	1:B:42:GLY:CA	2.69	0.69
1:A:97:LEU:CD2	1:A:101:LEU:CD2	2.58	0.69
1:B:323:TRP:CD1	1:B:324:MET:HE2	2.27	0.69
1:B:562:ARG:CG	1:B:562:ARG:NH1	2.36	0.69
1:A:38:ASP:C	1:A:38:ASP:OD1	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HA	1:A:299:GLU:OE1	1.92	0.68
1:A:565:TRP:C	1:A:566:LEU:CD2	2.66	0.68
1:B:73:HIS:CE1	1:B:103:ASP:HB3	2.29	0.67
1:B:33:GLU:HB3	1:B:34:LEU:CD2	2.23	0.67
1:A:71:GLN:O	1:A:71:GLN:HG2	1.95	0.66
1:A:27:LEU:O	1:A:30:ALA:CB	2.43	0.66
1:B:97:LEU:HD21	1:B:101:LEU:HD11	1.77	0.66
1:A:26:TRP:CH2	1:A:48:ARG:HD2	2.30	0.66
1:A:461:HIS:CD2	6:A:2131:HOH:O	2.48	0.66
1:A:24:VAL:O	1:A:28:MET:HG2	1.96	0.66
1:B:354:GLN:HE22	1:B:470:SER:HB2	1.61	0.65
1:A:523:PRO:HB3	3:A:1570:PEG:H42	1.78	0.65
1:A:255:THR:O	1:A:259:GLN:HG2	1.96	0.65
1:A:39:THR:OG1	1:A:40:THR:N	2.29	0.65
1:A:159:VAL:HG23	1:A:160:GLY:N	2.11	0.64
1:B:160:GLY:O	1:B:184:ARG:NH2	2.24	0.64
1:B:523:PRO:O	1:B:527:THR:HG23	1.98	0.64
1:A:383:PHE:CZ	1:A:439:MET:CE	2.81	0.64
1:B:146:VAL:O	1:B:150:GLN:HG3	1.98	0.64
1:A:562:ARG:C	1:A:562:ARG:CD	2.71	0.63
1:A:57:PRO:HG2	1:A:58:GLU:OE2	1.98	0.63
1:B:410:TRP:CH2	1:B:450:ARG:HB3	2.33	0.63
1:A:397:MET:HE2	1:A:458:LEU:CB	2.25	0.63
1:B:30:ALA:O	1:B:34:LEU:CG	2.39	0.63
1:A:408:VAL:CG2	1:A:435:ARG:O	2.47	0.63
1:A:545:MET:HE2	1:A:545:MET:HA	1.81	0.63
1:B:503:GLU:OE1	1:B:532:ARG:NH1	2.31	0.62
1:A:71:GLN:O	1:A:71:GLN:CG	2.48	0.61
1:B:296:GLY:O	1:B:297:ARG:HB2	2.00	0.61
1:B:412:LEU:CD1	1:B:439:MET:CE	2.78	0.61
1:A:213:ASN:H	1:A:213:ASN:ND2	1.95	0.61
1:A:408:VAL:HG22	1:A:435:ARG:O	2.00	0.61
1:B:323:TRP:HD1	1:B:324:MET:HE2	1.65	0.60
1:B:392:GLN:OE1	1:B:461:HIS:HD2	1.85	0.60
1:B:44:MET:O	1:B:48:ARG:HG2	2.01	0.60
1:A:354:GLN:HE22	1:A:470:SER:HB3	1.67	0.59
1:A:27:LEU:HB3	1:A:62:ARG:CD	2.30	0.58
1:B:97:LEU:HD22	1:B:113:ALA:CB	2.32	0.58
1:B:263:LEU:HD23	1:B:263:LEU:C	2.29	0.57
1:B:57:PRO:O	1:B:61:ALA:HB2	2.04	0.56
1:B:95:LEU:O	1:B:99:HIS:CE1	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:HIS:CD2	1:B:57:PRO:HD2	2.40	0.56
1:A:179:ALA:O	1:A:183:THR:HG23	2.06	0.56
1:B:27:LEU:HG	1:B:62:ARG:HD2	1.88	0.56
1:A:70:GLN:O	1:A:71:GLN:HB3	2.05	0.55
1:A:193:ARG:HD2	1:A:193:ARG:N	2.21	0.55
1:B:56:HIS:CD2	1:B:58:GLU:HB2	2.41	0.55
1:A:561:ARG:HG3	1:A:561:ARG:HH11	1.72	0.55
1:A:56:HIS:O	1:A:60:VAL:HG23	2.07	0.55
1:A:23:PHE:CG	1:A:53:HIS:HD2	2.25	0.55
1:A:277:HIS:CE1	1:A:281:HIS:CE1	2.92	0.55
1:B:97:LEU:CD2	1:B:101:LEU:CD1	2.68	0.55
1:A:562:ARG:CD	1:A:563:HIS:CD2	2.90	0.54
1:A:63:LEU:HD12	1:A:63:LEU:C	2.18	0.54
1:A:390:ASN:HB2	1:A:391:PRO:HD2	1.89	0.54
1:A:159:VAL:HG23	1:A:160:GLY:H	1.72	0.54
1:A:219:PRO:HB3	1:A:467:THR:HG21	1.90	0.54
1:A:134:TRP:CE3	1:A:137:ARG:HD2	2.43	0.54
1:A:297:ARG:CA	1:A:299:GLU:OE1	2.56	0.54
1:B:126:TYR:O	1:B:130:GLN:HG2	2.07	0.54
1:B:538[A]:ARG:NH2	6:B:2158:HOH:O	2.40	0.54
1:A:213:ASN:HD22	1:A:213:ASN:N	1.95	0.54
1:B:159:VAL:HG12	1:B:160:GLY:N	2.22	0.54
1:A:263:LEU:C	1:A:263:LEU:HD23	2.33	0.53
1:A:432:ASP:OD1	1:A:434:GLN:HG3	2.08	0.53
1:A:214:GLY:HA3	1:A:218:HIS:CD2	2.44	0.53
1:A:33:GLU:OE2	1:A:41:ALA:HB1	2.08	0.53
1:B:429:GLN:NE2	6:B:2125:HOH:O	2.41	0.53
1:B:297:ARG:HA	1:B:299:GLU:OE1	2.07	0.52
1:A:326:TYR:CE2	1:A:559:LEU:HD11	2.45	0.52
1:B:26:TRP:CZ3	1:B:48:ARG:HG3	2.45	0.52
1:B:240:MET:HG3	6:B:2041:HOH:O	2.10	0.52
1:A:44:MET:O	1:A:48:ARG:HG3	2.10	0.52
1:B:133:ASN:ND2	1:B:166:ALA:HB1	2.25	0.52
1:A:566:LEU:CD2	1:A:566:LEU:N	2.72	0.51
1:A:382:CYS:CB	1:A:397:MET:HE1	2.40	0.51
1:B:238:LEU:HB3	1:B:240:MET:HE2	1.91	0.51
1:B:80:LEU:C	1:B:82:GLN:N	2.66	0.51
1:A:58:GLU:OE2	1:A:58:GLU:N	2.43	0.51
1:B:55:GLY:O	1:B:56:HIS:C	2.52	0.51
1:A:159:VAL:HG23	1:A:161:ALA:N	2.17	0.51
1:A:66:VAL:O	1:A:69:THR:HB	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ASN:HB2	1:A:391:PRO:CD	2.41	0.50
1:A:368:ARG:NH1	1:A:377:GLY:O	2.44	0.50
1:B:80:LEU:O	1:B:81:GLN:C	2.55	0.50
1:A:218:HIS:CG	1:A:219:PRO:CD	2.91	0.50
1:A:560:ALA:C	1:A:562:ARG:N	2.65	0.50
1:B:63:LEU:C	1:B:65:ARG:N	2.68	0.50
1:B:70:GLN:O	1:B:71:GLN:CB	2.57	0.50
1:B:162:VAL:HG22	1:B:163:GLU:O	2.11	0.49
1:A:397:MET:CE	1:A:458:LEU:CB	2.87	0.49
1:B:70:GLN:O	1:B:71:GLN:HB2	2.11	0.49
1:A:334:LEU:CD1	1:A:342:TYR:CE2	2.95	0.49
1:A:218:HIS:ND1	1:A:219:PRO:HD2	2.28	0.49
1:B:57:PRO:HA	1:B:60:VAL:HB	1.94	0.48
1:A:564:GLY:O	1:A:566:LEU:HD21	2.12	0.48
1:B:354:GLN:OE1	1:B:466:HIS:ND1	2.46	0.48
1:A:383:PHE:CE2	1:A:439:MET:HE1	2.49	0.48
1:B:97:LEU:HD22	1:B:113:ALA:HB2	1.95	0.48
1:A:56:HIS:CD2	1:A:58:GLU:OE2	2.67	0.48
1:A:471:ASP:O	1:A:475:THR:HG23	2.13	0.48
1:A:290:ARG:NH2	1:A:293:GLY:O	2.47	0.47
1:B:499:LEU:HD13	1:B:542[A]:VAL:CG1	2.35	0.47
1:B:515:LYS:NZ	6:B:2155:HOH:O	2.45	0.47
1:A:193:ARG:H	1:A:193:ARG:CD	2.23	0.47
1:A:439:MET:HE2	1:A:450:ARG:HG3	1.96	0.47
1:A:159:VAL:CG2	1:A:160:GLY:N	2.78	0.47
1:A:203:LYS:HE2	1:A:566:LEU:HB2	1.96	0.47
1:A:408:VAL:HG23	1:A:435:ARG:O	2.15	0.47
1:B:57:PRO:O	1:B:61:ALA:CB	2.62	0.47
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.79	0.47
1:B:499:LEU:CD2	1:B:501:LEU:HD12	2.22	0.47
1:B:23:PHE:CZ	1:B:27:LEU:CD2	2.97	0.47
1:B:328:LEU:HD11	1:B:349:LEU:HG	1.97	0.47
1:B:66:VAL:O	1:B:69:THR:N	2.45	0.47
1:B:522:ASP:HA	1:B:523:PRO:HD2	1.76	0.47
1:A:27:LEU:O	1:A:30:ALA:CA	2.63	0.46
1:A:461:HIS:CD2	1:A:462:PRO:HA	2.49	0.46
1:B:64:GLY:N	1:B:79:LEU:HD13	2.30	0.46
1:A:55:GLY:O	1:A:56:HIS:C	2.59	0.46
1:B:23:PHE:CZ	1:B:27:LEU:HD22	2.50	0.46
1:B:29:LEU:O	1:B:29:LEU:HG	2.15	0.46
1:A:328:LEU:HD11	1:A:349:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:HIS:CD2	1:A:93:ILE:HD12	2.49	0.46
1:B:63:LEU:O	1:B:64:GLY:C	2.59	0.46
1:A:298:PRO:HA	6:A:2070:HOH:O	2.16	0.46
1:B:222:LEU:HD21	1:B:444:HIS:CE1	2.51	0.46
1:A:396:ARG:HG3	1:A:512:PHE:CE2	2.51	0.45
1:B:56:HIS:CD2	1:B:58:GLU:H	2.15	0.45
1:B:68:TRP:NE1	1:B:103:ASP:OD2	2.37	0.45
1:A:515:LYS:HA	1:A:515:LYS:HD3	1.82	0.45
1:A:404:VAL:HA	1:A:405:PRO:HD2	1.70	0.45
1:B:482:THR:HG22	1:B:506:VAL:HG23	1.99	0.45
1:B:120:LEU:C	1:B:121:LEU:HD23	2.41	0.45
1:B:311:ASN:OD1	1:B:311:ASN:C	2.59	0.45
1:B:354:GLN:OE1	1:B:466:HIS:CE1	2.71	0.44
2:A:1568:NHE:HC12	2:A:1568:NHE:H2'2	1.74	0.44
1:B:60:VAL:O	1:B:60:VAL:HG12	2.17	0.44
1:A:22:ASP:HB2	1:A:25:ALA:HB3	1.99	0.44
1:A:561:ARG:HG3	1:A:561:ARG:NH1	2.33	0.44
1:B:544[B]:HIS:HD2	1:B:547:GLY:N	2.08	0.44
1:A:121:LEU:HD13	1:A:124:GLU:HB2	1.98	0.44
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.33	0.44
1:B:392:GLN:HE21	1:B:392:GLN:HB3	1.48	0.44
1:B:44:MET:O	1:B:47:GLN:HB3	2.18	0.43
1:B:382:CYS:SG	1:B:397:MET:HE1	2.57	0.43
1:B:63:LEU:O	1:B:65:ARG:N	2.51	0.43
1:B:390:ASN:HB2	1:B:391:PRO:HD2	2.01	0.43
1:A:124:GLU:OE1	1:A:125:PRO:HD2	2.19	0.43
1:B:64:GLY:HA2	1:B:79:LEU:CD1	2.49	0.43
1:A:27:LEU:HB2	1:A:28:MET:HE2	2.00	0.43
1:A:72:ARG:HB3	1:A:75:GLU:OE1	2.19	0.42
1:B:417:GLU:O	1:B:418:ALA:C	2.58	0.42
1:A:233:ARG:HG2	1:A:233:ARG:HH21	1.85	0.42
1:A:562:ARG:O	1:A:562:ARG:CG	2.67	0.42
1:B:553:GLY:O	1:B:557:GLN:HG3	2.19	0.42
1:A:559:LEU:O	1:A:562:ARG:HB3	2.19	0.42
1:A:272:LEU:HG	1:A:276:LYS:HE3	2.02	0.42
1:B:123:GLU:O	1:B:125:PRO:HD3	2.19	0.42
1:B:80:LEU:C	1:B:82:GLN:H	2.28	0.42
1:B:97:LEU:HD23	1:B:101:LEU:HD12	1.96	0.42
1:B:297:ARG:N	1:B:298:PRO:HD3	2.35	0.42
1:B:327:VAL:HB	1:B:344:GLU:CG	2.50	0.42
1:B:165:PHE:CD2	1:B:165:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:TYR:CZ	1:A:559:LEU:HD11	2.56	0.41
1:A:121:LEU:HD22	1:A:123:GLU:HG2	2.01	0.41
1:B:323:TRP:CD1	1:B:324:MET:CE	3.01	0.41
1:B:327:VAL:HB	1:B:344:GLU:HG2	2.03	0.41
1:B:412:LEU:HD12	1:B:439:MET:CE	2.43	0.41
1:A:38:ASP:OD1	1:A:39:THR:N	2.53	0.41
1:B:133:ASN:HD21	1:B:166:ALA:CB	2.33	0.41
1:A:26:TRP:CZ3	1:A:48:ARG:HD2	2.55	0.41
1:A:90:HIS:CB	1:A:93:ILE:HD12	2.49	0.41
1:A:373:LEU:HB3	1:A:374:PRO:HD2	2.02	0.41
1:A:43:GLU:HG3	1:A:47:GLN:NE2	2.36	0.41
1:B:83:ALA:O	1:B:87:ALA:N	2.49	0.41
1:B:209:GLY:HA2	1:B:241:HIS:O	2.20	0.41
1:A:296:GLY:O	1:A:297:ARG:HB2	2.21	0.41
1:B:182:ARG:O	1:B:186:GLN:HG3	2.21	0.41
1:A:218:HIS:HD2	1:A:220:THR:H	1.59	0.41
1:A:36:MET:HE3	1:A:36:MET:HB3	1.97	0.41
1:A:63:LEU:HD12	1:A:66:VAL:HB	2.03	0.41
1:B:28:MET:HE2	1:B:28:MET:HB3	1.96	0.41
1:B:78:VAL:O	1:B:82:GLN:CG	2.41	0.41
1:B:133:ASN:HD21	1:B:166:ALA:HB1	1.86	0.41
1:B:202:SER:O	1:B:566:LEU:HB2	2.21	0.41
1:A:267:THR:O	1:A:268:ALA:HB3	2.21	0.41
1:A:159:VAL:CG2	1:A:160:GLY:H	2.33	0.40
1:A:560:ALA:C	1:A:562:ARG:H	2.28	0.40
1:B:62:ARG:O	1:B:65:ARG:HB3	2.22	0.40
1:B:83:ALA:O	1:B:86:ALA:HB3	2.21	0.40
1:B:297:ARG:CA	1:B:299:GLU:OE1	2.69	0.40
1:B:484:GLY:O	1:B:490:ARG:HD2	2.21	0.40
1:B:441:LYS:HA	1:B:441:LYS:HD2	1.84	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	546/568 (96%)	533 (98%)	12 (2%)	1 (0%)	43	44
1	B	549/568 (97%)	530 (96%)	19 (4%)	0	100	100
All	All	1095/1136 (96%)	1063 (97%)	31 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	THR

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	413/429 (96%)	392 (95%)	21 (5%)	21	21
1	B	416/429 (97%)	389 (94%)	27 (6%)	15	13
All	All	829/858 (97%)	781 (94%)	48 (6%)	18	16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	40	THR
1	A	89	GLU
1	A	97	LEU
1	A	101	LEU
1	A	121	LEU
1	A	162	VAL
1	A	206	LEU
1	A	213	ASN
1	A	233	ARG
1	A	259	GLN
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	299	GLU
1	A	368	ARG
1	A	379	VAL
1	A	389	LEU
1	A	417	GLU
1	A	485	GLU
1	A	515	LYS
1	A	555	LEU
1	A	566	LEU
1	B	21	GLN
1	B	27	LEU
1	B	34	LEU
1	B	47	GLN
1	B	71	GLN
1	B	84	SER
1	B	97	LEU
1	B	116	ARG
1	B	133	ASN
1	B	145	ASP
1	B	169	SER
1	B	233	ARG
1	B	298	PRO
1	B	304	ARG
1	B	311	ASN
1	B	334	LEU
1	B	344	GLU
1	B	368	ARG
1	B	379	VAL
1	B	392	GLN
1	B	403	GLU
1	B	408	VAL
1	B	447	TYR
1	B	466	HIS
1	B	526	LEU
1	B	534	ASP
1	B	562	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	56	HIS

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	130	GLN
1	A	150	GLN
1	A	213	ASN
1	A	218	HIS
1	A	239	GLN
1	A	271	HIS
1	A	277	HIS
1	A	281	HIS
1	A	354	GLN
1	A	392	GLN
1	A	461	HIS
1	A	544	HIS
1	B	56	HIS
1	B	99	HIS
1	B	133	ASN
1	B	281	HIS
1	B	385	ASN
1	B	392	GLN
1	B	434	GLN
1	B	461	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NHE	A	1568	-	13,13,13	1.89	3 (23%)	16,17,17	1.63	5 (31%)
2	NHE	B	1568	-	13,13,13	1.75	3 (23%)	16,17,17	1.21	2 (12%)
3	PEG	A	1569	-	6,6,6	0.71	0	5,5,5	0.70	0
2	NHE	B	1569	-	13,13,13	2.27	4 (30%)	16,17,17	2.38	3 (18%)
3	PEG	A	1570	-	6,6,6	0.63	0	5,5,5	1.50	1 (20%)

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	NHE	A	1568	-	-	2/7/15/15	0/1/1/1
2	NHE	B	1568	-	-	1/7/15/15	0/1/1/1
3	PEG	A	1569	-	-	3/4/4/4	-
2	NHE	B	1569	-	-	1/7/15/15	0/1/1/1
3	PEG	A	1570	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1568	NHE	C2-S	5.04	1.84	1.77
2	B	1569	NHE	C2-S	4.77	1.84	1.77
2	B	1569	NHE	O1-S	4.55	1.57	1.45
2	B	1569	NHE	O2-S	4.08	1.56	1.45
2	B	1568	NHE	O1-S	3.85	1.56	1.45
2	B	1568	NHE	C2-S	3.39	1.82	1.77
2	A	1568	NHE	O2-S	2.74	1.52	1.45
2	B	1568	NHE	O2-S	2.57	1.52	1.45
2	A	1568	NHE	O1-S	2.50	1.52	1.45
2	B	1569	NHE	O3-S	2.21	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1569	NHE	O1-S-C2	7.18	117.58	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1568	NHE	C5'-C6'-C1'	-3.46	104.89	111.09
2	B	1569	NHE	C6'-C1'-C2'	-3.37	104.98	110.80
3	A	1570	PEG	C3-O2-C2	-3.29	98.88	113.26
2	B	1568	NHE	O2-S-C2	2.84	111.02	106.73
2	A	1568	NHE	O3-S-O1	-2.63	104.82	111.40
2	A	1568	NHE	O3-S-C2	2.41	110.72	106.00
2	B	1569	NHE	C5'-C4'-C3'	-2.31	104.33	111.19
2	B	1568	NHE	O2-S-O1	-2.29	106.38	113.82
2	A	1568	NHE	C2-C1-N	-2.10	105.41	111.40
2	A	1568	NHE	O1-S-C2	2.03	109.80	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1568	NHE	C2'-C1'-N-C1
2	B	1569	NHE	N-C1-C2-S
3	A	1569	PEG	O1-C1-C2-O2
3	A	1570	PEG	C1-C2-O2-C3
3	A	1570	PEG	O1-C1-C2-O2
3	A	1569	PEG	C1-C2-O2-C3
2	A	1568	NHE	C2-C1-N-C1'
2	B	1568	NHE	C2-C1-N-C1'
3	A	1569	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1568	NHE	1	0
3	A	1570	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.