Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 08:54 pm BST

PDB ID	:	2VSY
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 (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 (1)) were used in the production of this report:

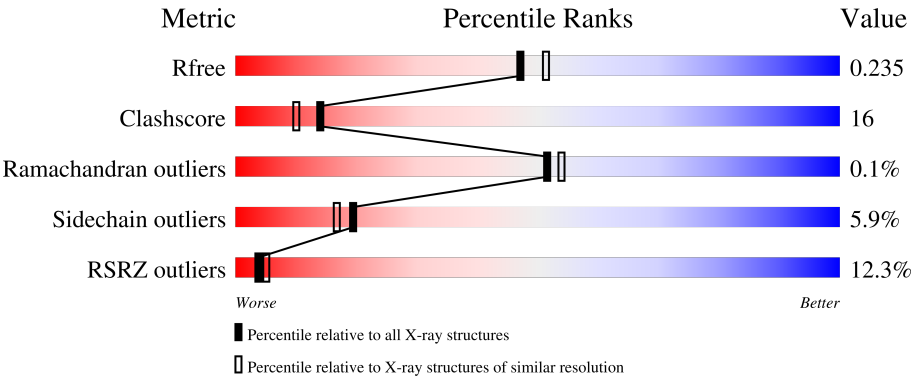
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	568	11% 74% 20%
1	B	568	13% 74% 20%

2 Entry composition (i)

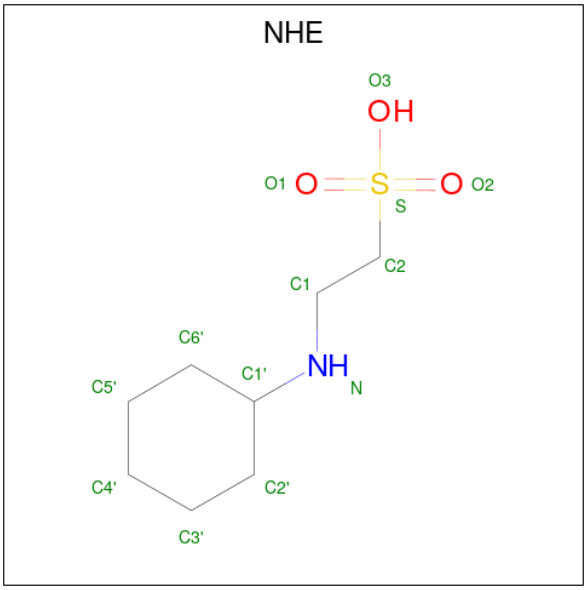
There are 6 unique types of molecules in this entry. The entry contains 8733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

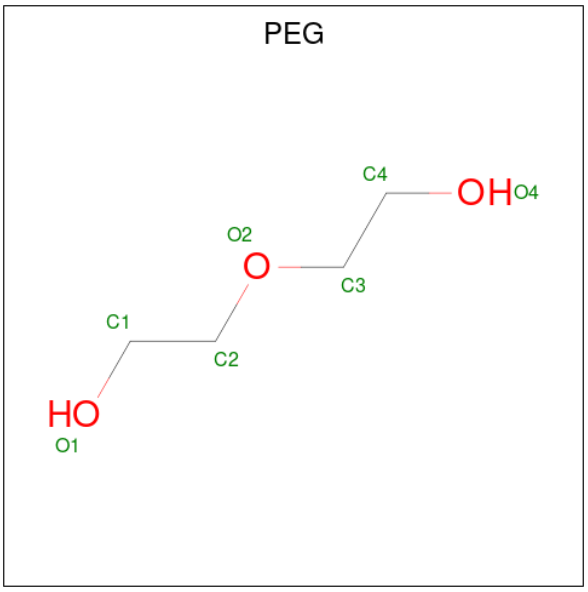
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	1	0
			4166	2632	770	748	16			
1	B	547	Total	C	N	O	S	0	4	0
			4189	2648	778	747	16			

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: 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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is PRASEODYMIUM ION (three-letter code: PR) (formula: Pr).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

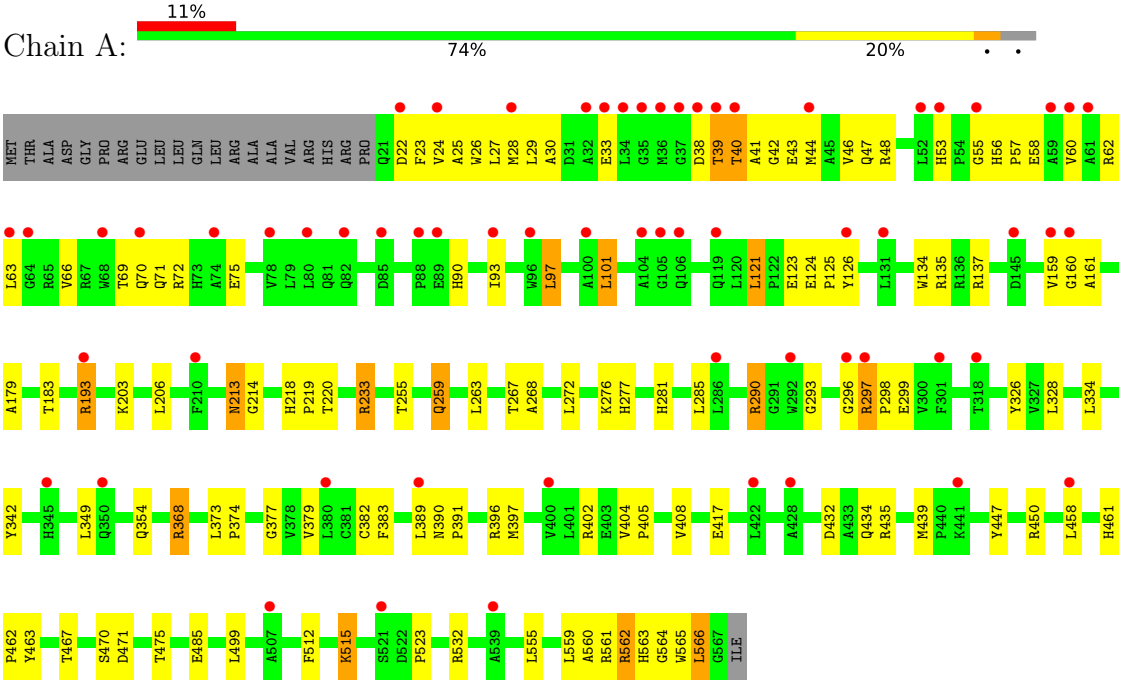
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	153	Total O 153 153	0	0
6	B	167	Total O 167 167	0	0

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 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.

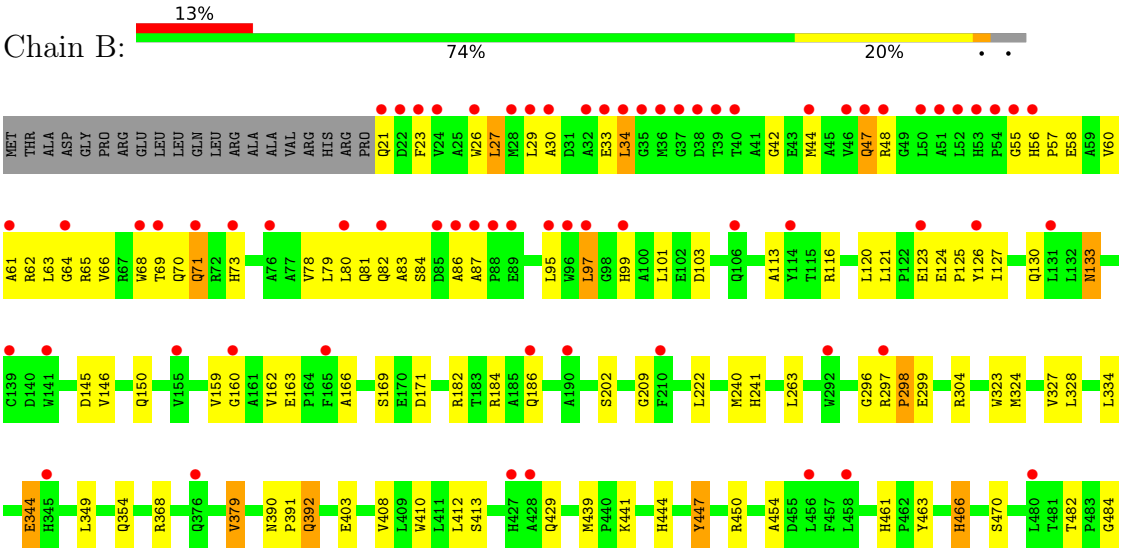
• Molecule 1: XCC0866

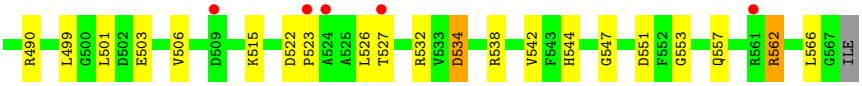
Chain A:



• Molecule 1: XCC0866

Chain B:




R490
L499
G500
L501
D502
E503
V506
D509
K515
D522
P523
A524
A525
L526
T527
R532
V533
D534
R538
V542
F543
H544
G547
D551
F552
G553
Q557
R561
R562
L566
G567
ILE

4 Data and refinement statistics (i)

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 19.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.10) 93.4 (19.97-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.193 , 0.236 0.194 , 0.235	Depositor DCC
R_{free} test set	1399 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 71.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
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.*

[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: PEG, NHE, CL, PR

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	0.69	0/4278	0.80	7/5839 (0.1%)
1	B	0.76	0/4311	0.80	2/5882 (0.0%)
All	All	0.73	0/8589	0.80	9/11721 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	A	290	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	290	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	368	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	368	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	A	402	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	A	499	LEU	CA-CB-CG	5.27	127.41	115.30
1	B	534	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	B	551	ASP	CB-CG-OD1	5.04	122.83	118.30

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	132	0
1	B	4189	0	4124	128	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	261	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 (261) 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: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:A:555:LEU:HD23	1:A:555:LEU:C	1.68	1.14
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: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: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:B:97:LEU:C	1:B:97:LEU:CD2	2.37	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:LEU:HD13	1:B:542[A]:VAL:HG11	1.57	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
1:A:555:LEU:C	1:A:555:LEU:CD2	2.47	0.82
1:A:565:TRP:O	1:A:566:LEU:HD22	1.80	0.81
1:A:218:HIS:CG	1:A:219:PRO:HD2	2.18	0.79
1:A:383:PHE:CZ	1:A:439:MET:HE3	2.18	0.79
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:A:565:TRP:C	1:A:566:LEU:HD22	2.04	0.77
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: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:A:562:ARG:HD3	1:A:562:ARG:C	2.06	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:33:GLU:C	1:B:34:LEU:HD23	2.08	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:HE1	1:A:458:LEU:HB2	1.69	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:323:TRP:CD1	1:B:324:MET:HE2	2.28	0.69
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:562:ARG:CG	1:B:562:ARG:NH1	2.36	0.69
1:A:297:ARG:HA	1:A:299:GLU:OE1	1.92	0.68
1:B:323:TRP:HD1	1:B:324:MET:HE2	1.59	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:B:439:MET:HE3	1:B:447:TYR:HD1	1.61	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:38:ASP:C	1:A:38:ASP:OD1	2.37	0.63
1:A:565:TRP:C	1:A:566:LEU:CD2	2.66	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:HD12	1:B:439:MET:HE2	1.84	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:A:562:ARG:C	1:A:562:ARG:CD	2.71	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
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:B:439:MET:CE	1:B:447:TYR:HD1	2.19	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: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:B:412:LEU:CD1	1:B:439:MET:HE2	2.36	0.53
1:A:432:ASP:OD1	1:A:434:GLN:HG3	2.08	0.53
1:A:397:MET:CE	1:A:458:LEU:CB	2.87	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:263:LEU:HD23	1:B:263:LEU:C	2.29	0.52
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:A:397:MET:HE2	1:A:458:LEU:CB	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:397:MET:HE2	1:A:458:LEU:HB3	1.92	0.51
1:A:58:GLU:OE2	1:A:58:GLU:N	2.43	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
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:A:218:HIS:CG	1:A:219:PRO:CD	2.91	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: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:80:LEU:C	1:B:82:GLN:N	2.66	0.48
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:263:LEU:C	1:A:263:LEU:HD23	2.33	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:A:193:ARG:H	1:A:193:ARG:CD	2.23	0.47
1:B:439:MET:HE3	1:B:447:TYR:CD1	2.45	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:B:23:PHE:CZ	1:B:27:LEU:HD22	2.50	0.46
1:B:55:GLY:O	1:B:56:HIS:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:90:HIS:CD2	1:A:93:ILE:HD12	2.49	0.46
1:B:412:LEU:HD12	1:B:439:MET:CE	2.43	0.46
1:B:439:MET:HE3	6:B:2129:HOH:O	2.16	0.46
1:A:298:PRO:HA	6:A:2070:HOH:O	2.16	0.46
1:A:560:ALA:C	1:A:562:ARG:N	2.65	0.46
1:B:222:LEU:HD21	1:B:444:HIS:CE1	2.51	0.46
1:B:80:LEU:O	1:B:81:GLN:C	2.55	0.45
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:383:PHE:CE2	1:A:439:MET:HE1	2.52	0.45
1:A:404:VAL:HA	1:A:405:PRO:HD2	1.70	0.45
1:B:63:LEU:C	1:B:65:ARG:N	2.68	0.45
1:B:482:THR:HG22	1:B:506:VAL:HG23	1.99	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:515:LYS:NZ	6:B:2155:HOH:O	2.45	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:A:439:MET:HE2	1:A:450:ARG:HG3	2.00	0.43
1:B:44:MET:O	1:B:47:GLN:HB3	2.18	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:72:ARG:HB3	1:A:75:GLU:OE1	2.19	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:412:LEU:CD1	1:B:439:MET:HE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:55:GLY:O	1:A:56:HIS:C	2.59	0.41
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: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:382:CYS:HB2	1:A:397:MET:CE	2.51	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:63:LEU:O	1:B:64:GLY:C	2.59	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:63:LEU:HD12	1:A:66:VAL:HB	2.03	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: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 (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	546/568 (96%)	533 (98%)	12 (2%)	1 (0%)	47 49
1	B	549/568 (97%)	530 (96%)	19 (4%)	0	100 100
All	All	1095/1136 (96%)	1063 (97%)	31 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	THR

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	413/429 (96%)	392 (95%)	21 (5%)	24 22
1	B	416/429 (97%)	388 (93%)	28 (7%)	16 13
All	All	829/858 (97%)	780 (94%)	49 (6%)	19 17

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	97	LEU
1	A	101	LEU
1	A	121	LEU
1	A	193	ARG
1	A	206	LEU
1	A	213	ASN
1	A	233	ARG
1	A	259	GLN
1	A	285	LEU
1	A	297	ARG

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Mol	Chain	Res	Type
1	A	379	VAL
1	A	389	LEU
1	A	417	GLU
1	A	447	TYR
1	A	463	TYR
1	A	485	GLU
1	A	515	LYS
1	A	532	ARG
1	A	562	ARG
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	171	ASP
1	B	298	PRO
1	B	304	ARG
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	413	SER
1	B	447	TYR
1	B	463	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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	53	HIS
1	A	56	HIS
1	A	82	GLN
1	A	150	GLN
1	A	213	ASN
1	A	218	HIS
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	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 monosaccharides 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	1.87	3 (23%)	16,17,17	1.70	5 (31%)
3	PEG	A	1569	-	6,6,6	0.71	0	5,5,5	0.71	0
2	NHE	B	1569	-	13,13,13	2.22	4 (30%)	16,17,17	2.73	4 (25%)
3	PEG	A	1570	-	6,6,6	0.62	0	5,5,5	1.52	1 (20%)
2	NHE	B	1568	-	13,13,13	1.72	3 (23%)	16,17,17	1.34	2 (12%)

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
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	-
2	NHE	B	1568	-	-	1/7/15/15	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1568	NHE	C2-S	5.03	1.84	1.77
2	B	1569	NHE	C2-S	4.77	1.84	1.77
2	B	1569	NHE	O1-S	4.38	1.57	1.45
2	B	1569	NHE	O2-S	3.93	1.56	1.45
2	B	1568	NHE	O1-S	3.71	1.56	1.45
2	B	1568	NHE	C2-S	3.40	1.82	1.77
2	A	1568	NHE	O2-S	2.65	1.52	1.45
2	B	1568	NHE	O2-S	2.49	1.52	1.45
2	A	1568	NHE	O1-S	2.42	1.52	1.45
2	B	1569	NHE	O3-S	2.21	1.55	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1569	NHE	O1-S-C2	8.86	117.58	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1568	NHE	O2-S-C2	3.41	111.02	106.92
2	B	1569	NHE	C6'-C1'-C2'	-3.37	104.98	110.82
3	A	1570	PEG	C3-O2-C2	-3.33	98.88	113.29
2	A	1568	NHE	C5'-C6'-C1'	-3.30	104.89	111.11
2	A	1568	NHE	O3-S-C2	3.06	110.72	105.77
2	A	1568	NHE	O3-S-O1	-2.64	104.82	111.27
2	A	1568	NHE	O1-S-C2	2.39	109.80	106.92
2	B	1569	NHE	C5'-C4'-C3'	-2.22	104.33	111.18
2	B	1568	NHE	O2-S-O1	-2.19	106.38	113.95
2	B	1569	NHE	O3-S-O2	2.09	116.39	111.27
2	A	1568	NHE	C2-C1-N	-2.06	105.41	111.25

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

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	547/568 (96%)	0.74	62 (11%)	5 6	29, 38, 48, 58	2 (0%)
1	B	547/568 (96%)	0.82	73 (13%)	3 4	28, 38, 49, 60	2 (0%)
All	All	1094/1136 (96%)	0.78	135 (12%)	4 5	28, 38, 48, 60	4 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	GLY	7.8
1	B	29	LEU	7.5
1	B	35	GLY	7.4
1	B	38	ASP	7.3
1	B	55	GLY	7.0
1	A	35	GLY	6.5
1	B	68	TRP	6.4
1	A	38	ASP	6.3
1	A	55	GLY	5.8
1	B	24	VAL	5.6
1	B	51	ALA	5.5
1	A	24	VAL	5.5
1	B	89	GLU	5.4
1	A	68	TRP	5.4
1	B	54	PRO	5.0
1	A	28	MET	4.9
1	B	190	ALA	4.8
1	A	88	PRO	4.8
1	A	159	VAL	4.7
1	B	28	MET	4.7
1	A	70	GLN	4.6
1	A	296	GLY	4.5
1	A	40	THR	4.5
1	A	39	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	4.4
1	B	80	LEU	4.4
1	A	104	ALA	4.3
1	B	160	GLY	4.3
1	B	53	HIS	4.2
1	B	21	GLN	4.2
1	B	22	ASP	4.1
1	B	39	THR	4.1
1	B	69	THR	4.1
1	A	34	LEU	4.1
1	A	33	GLU	4.0
1	B	36	MET	4.0
1	A	32	ALA	3.9
1	A	193	ARG	3.9
1	B	123	GLU	3.9
1	B	126	TYR	3.8
1	B	30	ALA	3.8
1	B	64	GLY	3.8
1	A	80	LEU	3.8
1	A	61	ALA	3.7
1	B	86	ALA	3.7
1	B	297	ARG	3.7
1	B	40	THR	3.7
1	B	48	ARG	3.7
1	B	26	TRP	3.7
1	B	376	GLN	3.6
1	B	87	ALA	3.6
1	A	22	ASP	3.5
1	B	292	TRP	3.5
1	A	428	ALA	3.5
1	B	46	VAL	3.4
1	B	82	GLN	3.4
1	B	50	LEU	3.3
1	A	82	GLN	3.3
1	A	36	MET	3.2
1	A	85	ASP	3.2
1	B	88	PRO	3.2
1	A	286	LEU	3.1
1	A	44	MET	3.0
1	A	63	LEU	3.0
1	B	32	ALA	3.0
1	A	458	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	3.0
1	A	507	ALA	3.0
1	B	73	HIS	2.9
1	A	292	TRP	2.9
1	B	97	LEU	2.9
1	B	47	GLN	2.8
1	A	64	GLY	2.8
1	B	71	GLN	2.8
1	B	56	HIS	2.8
1	A	37	GLY	2.8
1	A	106	GLN	2.8
1	B	96	TRP	2.8
1	B	523	PRO	2.8
1	A	105	GLY	2.7
1	B	131	LEU	2.7
1	B	524	ALA	2.7
1	A	78	VAL	2.7
1	A	301	PHE	2.7
1	B	509	ASP	2.6
1	B	61	ALA	2.6
1	A	89	GLU	2.6
1	B	456	LEU	2.6
1	A	93	ILE	2.5
1	A	96	TRP	2.5
1	A	297	ARG	2.5
1	B	186	GLN	2.5
1	A	119	GLN	2.5
1	B	527	THR	2.4
1	B	85	ASP	2.4
1	A	131	LEU	2.4
1	A	441	LYS	2.4
1	A	521	SER	2.4
1	A	52	LEU	2.4
1	A	389	LEU	2.4
1	B	34	LEU	2.4
1	A	60	VAL	2.4
1	B	99	HIS	2.3
1	A	53	HIS	2.3
1	A	380	LEU	2.3
1	B	561[A]	ARG	2.3
1	B	458	LEU	2.2
1	A	318	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	44	MET	2.2
1	B	428	ALA	2.2
1	B	480	LEU	2.2
1	A	210	PHE	2.2
1	B	33	GLU	2.2
1	B	210	PHE	2.2
1	A	400	VAL	2.2
1	A	345	HIS	2.1
1	A	160	GLY	2.1
1	B	76	ALA	2.1
1	A	422	LEU	2.1
1	B	141	TRP	2.1
1	B	106	GLN	2.1
1	A	74	ALA	2.1
1	A	145	ASP	2.1
1	B	95	LEU	2.1
1	A	100	ALA	2.1
1	B	23	PHE	2.1
1	B	114	TYR	2.1
1	B	165	PHE	2.1
1	A	350	GLN	2.0
1	A	126	TYR	2.0
1	A	539	ALA	2.0
1	B	345	HIS	2.0
1	B	155	VAL	2.0
1	B	427	HIS	2.0
1	B	139	CYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{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	NHE	B	1569	13/13	0.86	0.28	34,46,48,48	0
3	PEG	A	1570	7/7	0.87	0.18	51,52,53,55	0
4	PR	A	1572	1/1	0.92	0.07	54,54,54,54	1
3	PEG	A	1569	7/7	0.94	0.23	48,51,58,58	0
5	CL	B	1570	1/1	0.94	0.06	66,66,66,66	0
5	CL	B	1571	1/1	0.94	0.10	72,72,72,72	0
2	NHE	A	1568	13/13	0.97	0.13	36,41,43,44	0
2	NHE	B	1568	13/13	0.97	0.19	37,38,42,42	0
4	PR	A	1571	1/1	0.99	0.11	36,36,36,36	1
4	PR	B	1572	1/1	0.99	0.13	57,57,57,57	1

6.5 Other polymers (i)

There are no such residues in this entry.