



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VSY
Title : XANTHOMONAS CAMPESTRIS PUTATIVE OGT (XCC0866), APOS-
STRUCTURE
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

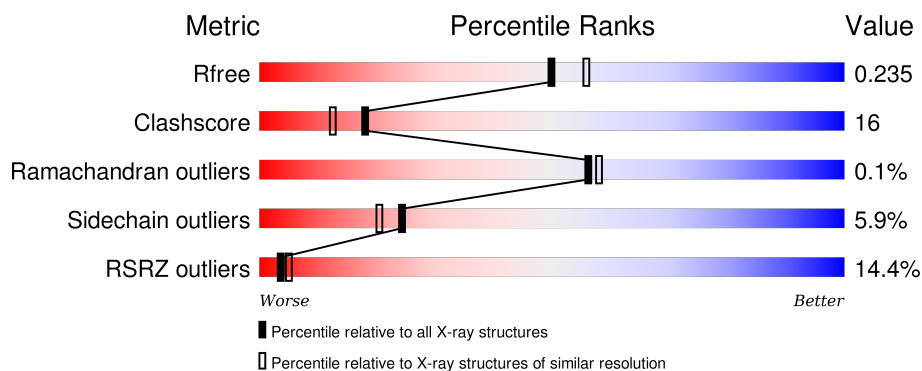
1 Overall quality at a glance

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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	
1	B	568	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NHE	B	1568	-	-	-	X
3	PEG	A	1569	-	-	-	X

2 Entry composition [i](#)

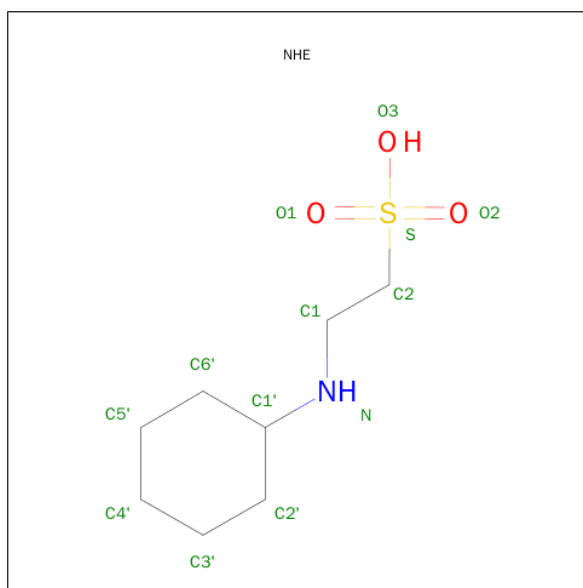
There are 6 unique types of molecules in this entry. The entry contains 8733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

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

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

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

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

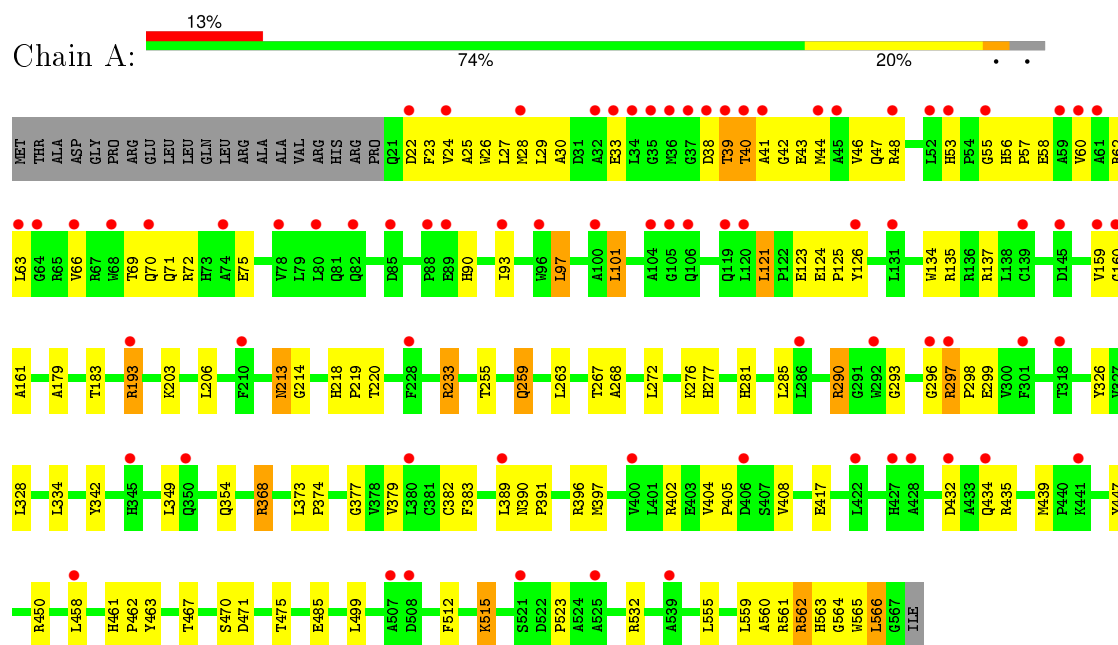
- Molecule 6 is water.

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

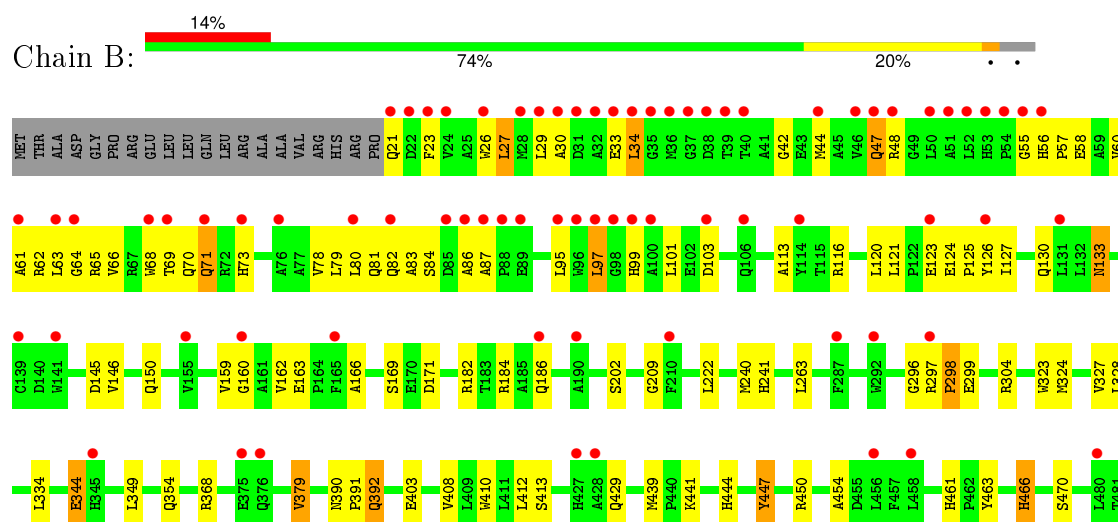
3 Residue-property plots [i](#)

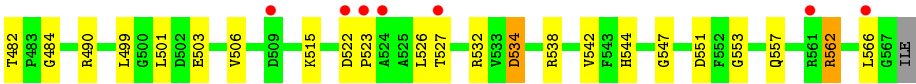
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: XCC0866



• Molecule 1: XCC0866





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.193 , 0.236 0.194 , 0.235	Depositor DCC
R_{free} test set	1399 reflections (2.04%)	DCC
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 , 72.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70018 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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(°)	Ideal(°)
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:HD23	1:B:34:LEU:N	1.55	1.16
1:B:78:VAL:O	1:B:82:GLN:HG3	1.47	1.15
1:A:555:LEU:C	1:A:555:LEU:HD23	1.68	1.14
1:B:562:ARG:CG	1:B:562:ARG:HH11	1.63	1.10
1:B:562:ARG:HG2	1:B:562:ARG:HH11	1.16	1.08
1:B:97:LEU:O	1:B:97:LEU:HD23	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:O	1:A:555:LEU:HD23	1.61	0.97
1:A:63:LEU:O	1:A:63:LEU:HD12	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:CD2	1:B:34:LEU:N	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:B:34:LEU:CD2	1:B:42:GLY:HA3	2.06	0.84
1:A:213:ASN:HD22	1:A:213:ASN:H	1.26	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:CD2	1:A:555:LEU:C	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:B:34:LEU:HD21	1:B:42:GLY:CA	2.15	0.75
1:A:562:ARG:HD2	1:A:563:HIS:CD2	2.21	0.75
1:A:562:ARG:C	1:A:562:ARG:HD3	2.06	0.74
1:B:33:GLU:C	1:B:34:LEU:HD23	2.08	0.74
1:B:33:GLU:HB3	1:B:34:LEU:HD23	1.69	0.74
1:A:461:HIS:HD2	6:A:2131:HOH:O	1.69	0.74
1:B:544[B]:HIS:HD2	1:B:547:GLY:H	1.35	0.73
1:B:34:LEU:H	1:B:34:LEU:HD23	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:334:LEU:HD11	1:A:342:TYR:CE2	2.25	0.72
1:A:29:LEU:HG	1:A:33:GLU:OE1	1.89	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:CD	1:A:562:ARG:O	2.35	0.71
1:B:34:LEU:HD21	1:B:42:GLY:HA2	1.71	0.71
1:B:544[B]:HIS:CD2	1:B:547:GLY:H	2.08	0.71
1:B:73:HIS:ND1	1:B:103:ASP:HB3	2.05	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:HG3	1:B:562:ARG:HH11	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:461:HIS:CD2	6:A:2131:HOH:O	2.48	0.66
1:A:26:TRP:CH2	1:A:48:ARG:HD2	2.30	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:OD1	1:A:38:ASP:C	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:CG	1:A:71:GLN:O	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:ND2	1:A:213:ASN:H	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:CD	1:A:562:ARG:C	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:B:56:HIS:CD2	1:B:58:GLU:HB2	2.41	0.55
1:A:193:ARG:N	1:A:193:ARG:HD2	2.21	0.55
1:B:439:MET:CE	1:B:447:TYR:HD1	2.19	0.55
1:A:561:ARG:HH11	1:A:561:ARG:HG3	1.72	0.55
1:A:56:HIS:O	1:A:60:VAL:HG23	2.07	0.55
1:B:97:LEU:CD2	1:B:101:LEU:CD1	2.68	0.55
1:A:277:HIS:CE1	1:A:281:HIS:CE1	2.92	0.55
1:A:23:PHE:CG	1:A:53:HIS:HD2	2.25	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:297:ARG:CA	1:A:299:GLU:OE1	2.56	0.54
1:A:134:TRP:CE3	1:A:137:ARG:HD2	2.43	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:297:ARG:HA	1:B:299:GLU:OE1	2.07	0.52
1:B:263:LEU:C	1:B:263:LEU:HD23	2.29	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:N	1:A:566:LEU:CD2	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:B:97:LEU:HD22	1:B:113:ALA:HB2	1.95	0.48
1:A:263:LEU:C	1:A:263:LEU:HD23	2.33	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:B:499:LEU:HD13	1:B:542[A]:VAL:CG1	2.35	0.47
1:A:290:ARG:NH2	1:A:293:GLY:O	2.47	0.47
1:A:193:ARG:CD	1:A:193:ARG:H	2.23	0.47
1:B:439:MET:HE3	1:B:447:TYR:CD1	2.45	0.47
1:B:499:LEU:CD2	1:B:501:LEU:HD12	2.22	0.47
1:A:159:VAL:CG2	1:A:160:GLY:N	2.78	0.47
1:B:57:PRO:O	1:B:61:ALA:CB	2.62	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:62:ARG:HH11	1:B:62:ARG:HG3	1.79	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:55:GLY:O	1:B:56:HIS:C	2.52	0.46
1:B:23:PHE:CZ	1:B:27:LEU:HD22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HG	1:B:29:LEU:O	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: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:A:298:PRO:HA	6:A:2070:HOH:O	2.16	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:HD3	1:A:515:LYS:HA	1.82	0.45
1:A:383:PHE:CE2	1:A:439:MET:HE1	2.52	0.45
1:B:63:LEU:C	1:B:65:ARG:N	2.68	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:354:GLN:OE1	1:B:466:HIS:CE1	2.71	0.44
1:B:60:VAL:HG12	1:B:60:VAL:O	2.17	0.44
2:A:1568:NHE:HC12	2:A:1568:NHE:H2'2	1.74	0.44
1:A:22:ASP:HB2	1:A:25:ALA:HB3	1.99	0.44
1:A:561:ARG:NH1	1:A:561:ARG:HG3	2.33	0.44
1:B:544[B]:HIS:HD2	1:B:547:GLY:N	2.08	0.44
1:B:515:LYS:NZ	6:B:2155:HOH:O	2.45	0.44
1:A:121:LEU:HD13	1:A:124:GLU:HB2	1.98	0.44
1:B:392:GLN:HB3	1:B:392:GLN:HE21	1.48	0.44
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.33	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:562:ARG:CG	1:A:562:ARG:O	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:233:ARG:HG2	1:A:233:ARG:HH21	1.85	0.42
1:A:559:LEU:O	1:A:562:ARG:HB3	2.19	0.42
1:B:123:GLU:O	1:B:125:PRO:HD3	2.19	0.42
1:A:272:LEU:HG	1:A:276:LYS:HE3	2.02	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:90:HIS:CB	1:A:93:ILE:HD12	2.49	0.41
1:A:382:CYS:HB2	1:A:397:MET:CE	2.51	0.41
1:A:26:TRP:CZ3	1:A:48:ARG:HD2	2.55	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:209:GLY:HA2	1:B:241:HIS:O	2.20	0.41
1:B:83:ALA:O	1:B:87:ALA:N	2.49	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:B:78:VAL:O	1:B:82:GLN:CG	2.41	0.41
1:A:63:LEU:HD12	1:A:66:VAL:HB	2.03	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:297:ARG:CA	1:B:299:GLU:OE1	2.69	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:484:GLY:O	1:B:490:ARG:HD2	2.21	0.40
1:B:441:LYS:HD2	1:B:441:LYS:HA	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%)	52	53
1	B	549/568 (97%)	530 (96%)	19 (4%)	0	100	100
All	All	1095/1136 (96%)	1063 (97%)	31 (3%)	1 (0%)	56	58

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%)	29	26
1	B	416/429 (97%)	388 (93%)	28 (7%)	20	16
All	All	829/858 (97%)	780 (94%)	49 (6%)	24	20

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

Some 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 carbohydrates 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	-	12,13,13	1.25	2 (16%)	15,17,17	1.81	4 (26%)
3	PEG	A	1569	-	6,6,6	0.71	0	5,5,5	0.70	0
3	PEG	A	1570	-	6,6,6	0.63	0	5,5,5	1.53	1 (20%)
2	NHE	B	1568	-	12,13,13	1.55	3 (25%)	15,17,17	1.54	1 (6%)
2	NHE	B	1569	-	12,13,13	1.91	3 (25%)	15,17,17	3.73	7 (46%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1568	NHE	O1-S	2.21	1.52	1.45
2	B	1568	NHE	O2-S	2.27	1.52	1.45
2	A	1568	NHE	O2-S	2.43	1.52	1.45
2	B	1568	NHE	O3-S	2.86	1.53	1.46
2	B	1568	NHE	O1-S	3.44	1.56	1.45
2	B	1569	NHE	O3-S	3.51	1.55	1.46
2	B	1569	NHE	O2-S	3.65	1.56	1.45
2	B	1569	NHE	O1-S	4.07	1.57	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1568	NHE	C5'-C6'-C1'	-4.04	104.89	111.13
2	B	1569	NHE	C6'-C1'-C2'	-3.43	104.98	110.82
3	A	1570	PEG	C3-O2-C2	-3.36	98.88	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1569	NHE	C1-C2-S	-3.05	105.50	113.73
2	A	1568	NHE	O3-S-O1	-2.92	104.82	111.61
2	B	1569	NHE	O2-S-C2	-2.50	104.77	106.91
2	B	1569	NHE	C5'-C4'-C3'	-2.17	104.33	111.27
2	B	1569	NHE	O3-S-O1	-2.00	106.94	111.61
2	A	1568	NHE	C2-C1-N	-2.00	105.41	111.32
2	B	1569	NHE	O3-S-O2	2.05	116.39	111.61
2	A	1568	NHE	O1-S-C2	3.39	109.80	106.91
2	B	1568	NHE	O2-S-C2	4.82	111.02	106.91
2	B	1569	NHE	O1-S-C2	12.52	117.58	106.91

There are no chirality outliers.

There are no torsion outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	547/568 (96%)	0.82	75 (13%) 4 5	29, 38, 48, 58	2 (0%)
1	B	547/568 (96%)	0.90	82 (14%) 3 5	28, 38, 49, 60	2 (0%)
All	All	1094/1136 (96%)	0.86	157 (14%) 3 5	28, 38, 48, 60	4 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	GLY	8.1
1	B	29	LEU	7.8
1	B	35	GLY	7.7
1	B	38	ASP	7.5
1	B	55	GLY	7.2
1	A	35	GLY	6.8
1	B	68	TRP	6.8
1	A	38	ASP	6.5
1	B	24	VAL	6.0
1	B	51	ALA	5.8
1	A	55	GLY	5.8
1	A	24	VAL	5.8
1	A	68	TRP	5.7
1	B	89	GLU	5.5
1	B	190	ALA	5.1
1	A	159	VAL	5.0
1	A	28	MET	5.0
1	B	54	PRO	5.0
1	A	88	PRO	4.9
1	A	70	GLN	4.8
1	A	296	GLY	4.8
1	B	28	MET	4.7
1	A	39	THR	4.6
1	A	40	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	4.6
1	B	52	LEU	4.6
1	B	80	LEU	4.6
1	B	160	GLY	4.4
1	B	22	ASP	4.4
1	B	21	GLN	4.3
1	B	53	HIS	4.2
1	B	39	THR	4.2
1	B	69	THR	4.2
1	A	34	LEU	4.2
1	B	36	MET	4.1
1	B	123	GLU	4.1
1	A	193	ARG	4.1
1	B	126	TYR	4.0
1	A	32	ALA	4.0
1	B	30	ALA	4.0
1	B	86	ALA	4.0
1	B	64	GLY	4.0
1	A	61	ALA	4.0
1	A	80	LEU	4.0
1	A	33	GLU	3.9
1	B	40	THR	3.9
1	B	48	ARG	3.9
1	B	26	TRP	3.9
1	A	428	ALA	3.8
1	B	292	TRP	3.8
1	B	297	ARG	3.8
1	B	87	ALA	3.8
1	B	376	GLN	3.7
1	A	22	ASP	3.7
1	B	46	VAL	3.5
1	A	36	MET	3.4
1	B	50	LEU	3.4
1	B	82	GLN	3.4
1	A	85	ASP	3.4
1	A	82	GLN	3.4
1	B	88	PRO	3.3
1	A	63	LEU	3.3
1	A	59	ALA	3.2
1	B	32	ALA	3.2
1	A	286	LEU	3.2
1	A	458	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	507	ALA	3.1
1	A	44	MET	3.1
1	A	64	GLY	3.1
1	B	97	LEU	3.0
1	A	292	TRP	3.0
1	B	73	HIS	3.0
1	B	71	GLN	3.0
1	A	105	GLY	3.0
1	A	106	GLN	3.0
1	B	56	HIS	2.9
1	B	96	TRP	2.9
1	B	47	GLN	2.9
1	B	131	LEU	2.9
1	A	37	GLY	2.9
1	B	61	ALA	2.9
1	A	78	VAL	2.9
1	B	523	PRO	2.9
1	A	93	ILE	2.8
1	A	301	PHE	2.8
1	B	524	ALA	2.8
1	B	509	ASP	2.8
1	A	89	GLU	2.8
1	B	456	LEU	2.7
1	B	34	LEU	2.6
1	B	186	GLN	2.6
1	A	297	ARG	2.6
1	A	119	GLN	2.6
1	A	96	TRP	2.6
1	A	389	LEU	2.6
1	B	527	THR	2.6
1	A	52	LEU	2.5
1	A	131	LEU	2.5
1	A	60	VAL	2.5
1	A	441	LYS	2.5
1	B	85	ASP	2.5
1	A	521	SER	2.5
1	A	380	LEU	2.5
1	B	458	LEU	2.4
1	B	428	ALA	2.4
1	B	99	HIS	2.4
1	A	53	HIS	2.4
1	A	210	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	LEU	2.4
1	B	210	PHE	2.4
1	B	480	LEU	2.4
1	A	74	ALA	2.3
1	A	400	VAL	2.3
1	A	318	THR	2.3
1	B	44	MET	2.3
1	B	561[A]	ARG	2.3
1	B	76	ALA	2.3
1	B	33	GLU	2.3
1	A	422	LEU	2.3
1	A	160	GLY	2.3
1	B	114	TYR	2.2
1	B	141	TRP	2.2
1	A	539	ALA	2.2
1	B	23	PHE	2.2
1	A	345	HIS	2.2
1	A	45	ALA	2.2
1	A	100	ALA	2.2
1	A	145	ASP	2.2
1	B	155	VAL	2.2
1	B	98	GLY	2.2
1	B	31	ASP	2.2
1	A	228	PHE	2.2
1	B	165	PHE	2.2
1	A	350	GLN	2.2
1	B	106	GLN	2.1
1	A	126	TYR	2.1
1	A	41	ALA	2.1
1	B	566	LEU	2.1
1	B	522	ASP	2.1
1	A	525	ALA	2.1
1	B	100	ALA	2.1
1	B	139	CYS	2.1
1	B	287	PHE	2.1
1	A	120	LEU	2.1
1	A	139	CYS	2.1
1	A	406	ASP	2.1
1	A	508	ASP	2.1
1	B	375	GLU	2.0
1	A	427	HIS	2.0
1	B	345	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	63	LEU	2.0
1	A	432	ASP	2.0
1	B	103	ASP	2.0
1	A	434	GLN	2.0
1	B	427	HIS	2.0
1	A	48	ARG	2.0
1	A	66	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PEG	A	1569	7/7	0.94	0.22	2.30	48,51,58,58	0
2	NHE	B	1568	13/13	0.97	0.19	2.17	37,38,42,42	0
2	NHE	B	1569	13/13	0.86	0.28	1.79	34,46,48,48	0
3	PEG	A	1570	7/7	0.88	0.18	0.82	51,52,53,55	0
2	NHE	A	1568	13/13	0.97	0.13	-0.36	36,41,43,44	0
4	PR	B	1572	1/1	0.99	0.13	-	57,57,57,57	1
5	CL	B	1570	1/1	0.94	0.06	-	66,66,66,66	0
4	PR	A	1571	1/1	0.99	0.11	-	36,36,36,36	1
4	PR	A	1572	1/1	0.92	0.07	-	54,54,54,54	1
5	CL	B	1571	1/1	0.95	0.10	-	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.