



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:18 AM UTC

PDB ID : 3FNT / pdb_00003fnt
Title : Crystal structure of pepstatin A bound histo-aspartic protease (HAP) from Plasmodium falciparum
Authors : Bhaumik, P.; Gustchina, A.; Wlodawer, A.
Deposited on : 2008-12-26
Resolution : 3.30 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 : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

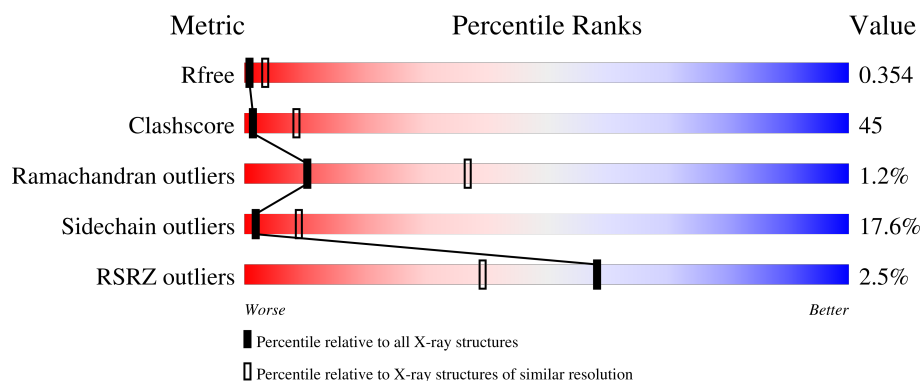
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	332	2% 32% 47% 16% • •
2	I	6	17% 17% 33% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2635 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 HAP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2570	1665	399	498	8			

- Molecule 2 is a protein called Inhibitor, (IVA)VV(STA)A(STA).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			48	34	5	9			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

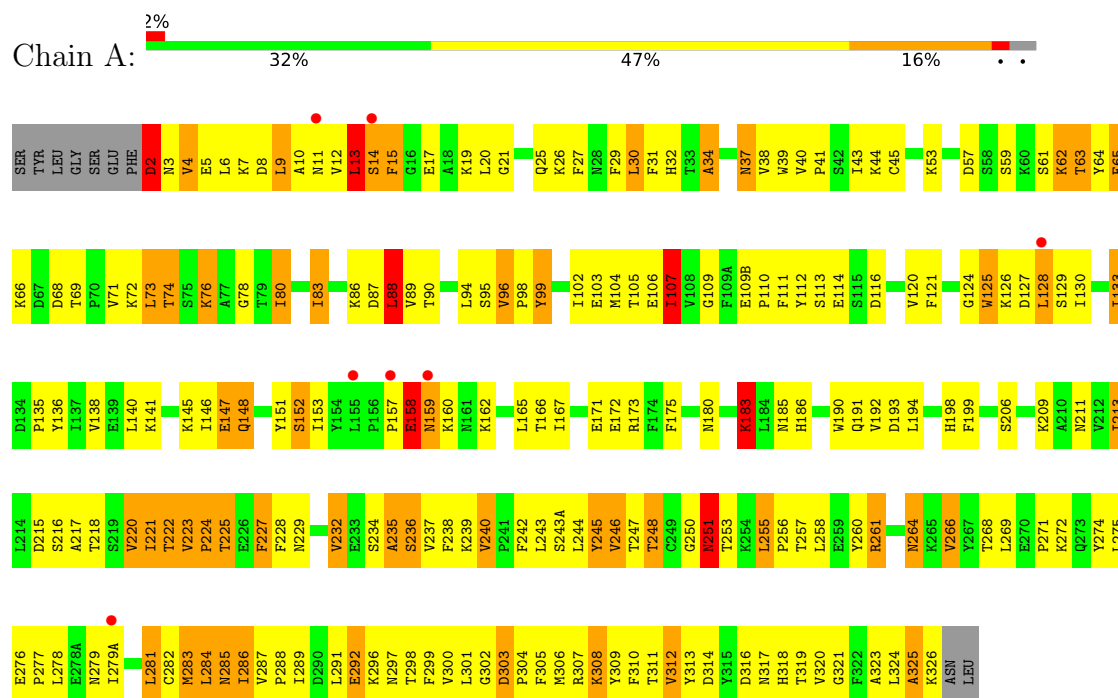
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

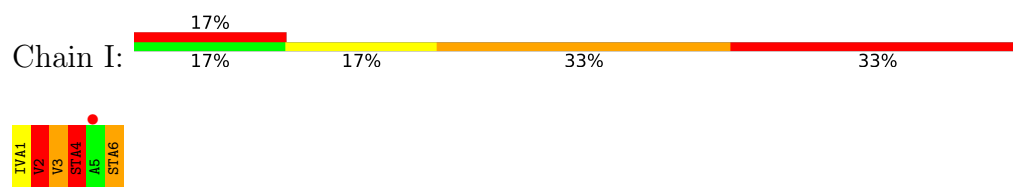
3 Residue-property plots

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 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: HAP protein



• Molecule 2: Inhibitor, (IVA)VV(STA)A(STA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.70Å 70.70Å 158.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.30 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.30) 99.2 (20.00-3.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.4.0057	Depositor
R, R_{free}	0.285 , 0.353 0.285 , 0.354	Depositor DCC
R_{free} test set	368 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 8.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.170 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2635	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: IVA, STA, 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	1.45	24/2634 (0.9%)	1.44	34/3575 (1.0%)
2	I	0.85	0/17	2.18	1/21 (4.8%)
All	All	1.45	24/2651 (0.9%)	1.45	35/3596 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279(A)	ILE	CA-CB	9.85	1.65	1.54
1	A	14	SER	CA-CB	9.27	1.63	1.53
1	A	133	ILE	CA-CB	7.97	1.63	1.54
1	A	285	ASN	CA-C	-7.80	1.43	1.53
1	A	221	ILE	CA-CB	-7.66	1.45	1.54
1	A	279	ASN	CA-C	6.73	1.59	1.53
1	A	2	ASP	N-CA	6.43	1.58	1.46
1	A	261	ARG	N-CA	6.41	1.53	1.45
1	A	279(A)	ILE	CA-C	6.35	1.59	1.52
1	A	130	ILE	CA-CB	6.14	1.62	1.54
1	A	222	THR	CA-CB	-6.12	1.43	1.53
1	A	312	VAL	CA-CB	-6.10	1.46	1.54
1	A	180	ASN	CA-C	-6.10	1.45	1.52
1	A	74	THR	CA-CB	5.91	1.60	1.52
1	A	308	LYS	N-CA	5.69	1.52	1.46
1	A	222	THR	CA-C	-5.62	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	LEU	N-CA	-5.45	1.39	1.46
1	A	43	ILE	CA-CB	5.41	1.61	1.54
1	A	152	SER	N-CA	-5.40	1.39	1.46
1	A	96	VAL	CA-CB	5.39	1.61	1.54
1	A	286	ILE	N-CA	-5.25	1.39	1.46
1	A	223	VAL	CA-CB	-5.08	1.47	1.54
1	A	284	LEU	CA-C	-5.06	1.46	1.53
1	A	153	ILE	CA-CB	-5.05	1.47	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	TYR	N-CA-C	8.26	122.71	108.76
1	A	107	ILE	CB-CA-C	-8.05	98.32	110.55
1	A	246	VAL	N-CA-C	7.93	118.82	108.35
1	A	281	LEU	N-CA-C	7.61	121.30	108.90
1	A	255	LEU	CA-C-N	7.32	128.75	120.85
1	A	255	LEU	C-N-CA	7.32	128.75	120.85
1	A	240	VAL	CA-C-N	6.87	128.43	119.84
1	A	240	VAL	C-N-CA	6.87	128.43	119.84
1	A	227	PHE	N-CA-C	-6.81	103.79	111.07
1	A	312	VAL	CB-CA-C	-6.37	100.68	110.50
1	A	183	LYS	N-CA-C	6.32	118.58	108.41
1	A	141	LYS	N-CA-C	-6.31	103.68	112.45
1	A	88	LEU	N-CA-C	6.25	119.54	110.42
1	A	158	GLU	CB-CA-C	6.25	120.31	110.19
1	A	128	LEU	CA-CB-CG	6.13	137.77	116.30
1	A	325	ALA	N-CA-C	6.07	119.09	109.50
1	A	102	ILE	N-CA-C	6.06	116.59	107.80
1	A	145	LYS	N-CA-C	-5.81	107.43	114.75
1	A	276	GLU	CA-C-N	5.72	126.04	119.92
1	A	276	GLU	C-N-CA	5.72	126.04	119.92
2	I	3	VAL	CA-CB-CG2	5.59	119.90	110.40
1	A	266	VAL	N-CA-C	5.48	116.67	109.21
1	A	14	SER	CB-CA-C	5.43	119.95	111.70
1	A	236	SER	CB-CA-C	5.36	116.40	109.80
1	A	213	ILE	CB-CA-C	-5.35	102.52	110.33
1	A	251	ASN	N-CA-C	5.34	117.44	108.96
1	A	125	TRP	N-CA-C	5.30	117.47	109.41
1	A	281	LEU	CA-CB-CG	-5.29	97.79	116.30
1	A	13	LEU	N-CA-C	-5.18	99.50	108.52
1	A	147	GLU	N-CA-C	5.06	117.77	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ALA	CA-C-N	-5.05	114.73	122.87
1	A	34	ALA	C-N-CA	-5.05	114.73	122.87
1	A	285	ASN	N-CA-C	-5.03	104.07	111.81
1	A	69	THR	CA-C-N	5.01	124.92	119.76
1	A	69	THR	C-N-CA	5.01	124.92	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	4	STA	Mainchain,Peptide

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	2570	0	2523	230	3
2	I	48	0	60	7	0
3	A	8	0	12	0	0
4	A	9	0	0	3	0
All	All	2635	0	2595	234	3

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 45.

All (234) 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:7:LYS:HB2	1:A:15:PHE:CE2	1.75	1.21
1:A:7:LYS:HB2	1:A:15:PHE:HE2	1.07	1.08
1:A:289:ILE:HG22	1:A:291:LEU:HD12	1.30	1.05
1:A:303:ASP:HB3	1:A:307:ARG:HE	1.17	1.05
1:A:88:LEU:HD11	1:A:95:SER:HB3	1.07	1.05
1:A:183:LYS:HE3	1:A:183:LYS:HA	1.40	1.01
1:A:13:LEU:H	1:A:307:ARG:HH22	0.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:HD3	1:A:309:TYR:CE2	2.00	0.97
1:A:235:ALA:O	1:A:237:VAL:HG23	1.66	0.95
1:A:135:PRO:HG2	1:A:138:VAL:HG23	1.46	0.95
1:A:88:LEU:CD1	1:A:95:SER:HB3	1.98	0.92
1:A:13:LEU:H	1:A:307:ARG:NH2	1.67	0.92
1:A:232:VAL:HA	1:A:235:ALA:HB3	1.51	0.92
2:I:2:VAL:HG12	2:I:4:STA:HD21	1.49	0.91
1:A:251:ASN:HB3	1:A:255:LEU:HD12	1.51	0.90
1:A:229:ASN:HA	1:A:232:VAL:HG12	1.50	0.90
1:A:7:LYS:CB	1:A:15:PHE:HE2	1.83	0.90
1:A:32:HIS:HD2	1:A:34:ALA:H	1.15	0.89
1:A:289:ILE:HG22	1:A:291:LEU:CD1	2.04	0.88
1:A:32:HIS:CD2	1:A:34:ALA:H	1.94	0.86
1:A:324:LEU:HG	1:A:325:ALA:H	1.41	0.84
1:A:239:LYS:HZ2	1:A:245:TYR:HE1	1.28	0.82
1:A:88:LEU:HD11	1:A:95:SER:CB	2.01	0.81
1:A:239:LYS:NZ	1:A:245:TYR:CE1	2.48	0.81
1:A:220:VAL:HG13	1:A:285:ASN:O	1.82	0.78
1:A:303:ASP:N	1:A:304:PRO:HD2	1.98	0.78
1:A:13:LEU:N	1:A:307:ARG:HH22	1.80	0.78
1:A:9:LEU:HD11	1:A:116:ASP:H	1.48	0.77
1:A:14:SER:O	1:A:30:LEU:HD12	1.84	0.77
1:A:27:PHE:HB2	1:A:29:PHE:CE1	2.19	0.77
1:A:193:ASP:OD2	1:A:209:LYS:HG2	1.85	0.75
1:A:109(B):GLU:OE2	1:A:112:TYR:HB3	1.86	0.75
1:A:199:PHE:CE1	1:A:258:LEU:HG	2.22	0.75
1:A:107:ILE:HD12	1:A:107:ILE:H	1.52	0.75
1:A:152:SER:O	1:A:165:LEU:HD12	1.87	0.75
1:A:88:LEU:HA	1:A:96:VAL:O	1.86	0.74
1:A:89:VAL:CG2	1:A:99:TYR:HB3	2.18	0.74
1:A:216:SER:HB3	1:A:306:MET:HE1	1.70	0.73
1:A:152:SER:HB2	1:A:310:PHE:CZ	2.22	0.73
1:A:228:PHE:CE1	1:A:288:PRO:HD3	2.23	0.73
1:A:240:VAL:HB	1:A:244:LEU:HD13	1.70	0.72
1:A:62:LYS:NZ	1:A:62:LYS:HB2	2.03	0.71
1:A:314:ASP:OD2	1:A:317:ASN:HB2	1.91	0.71
1:A:17:GLU:OE2	1:A:26:LYS:HD3	1.89	0.71
1:A:220:VAL:HG11	1:A:287:VAL:HG12	1.72	0.71
1:A:147:GLU:HG3	1:A:148:GLN:H	1.56	0.70
1:A:89:VAL:HG21	1:A:99:TYR:HB3	1.75	0.69
1:A:135:PRO:O	1:A:136:TYR:C	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:CE1	1:A:313:TYR:HB2	2.27	0.69
1:A:284:LEU:HD12	1:A:284:LEU:H	1.56	0.69
1:A:292:GLU:HG2	1:A:296:LYS:H	1.58	0.69
1:A:78:GLY:HA3	1:A:109:GLY:HA3	1.75	0.68
1:A:110:PRO:HD2	1:A:111:PHE:CE2	2.28	0.68
1:A:2:ASP:N	1:A:167:ILE:O	2.26	0.68
1:A:63:THR:HB	1:A:87:ASP:OD1	1.93	0.67
1:A:183:LYS:HE3	1:A:183:LYS:CA	2.21	0.66
1:A:303:ASP:CG	1:A:307:ARG:HH21	2.03	0.65
1:A:90:THR:HA	1:A:94:LEU:O	1.96	0.65
1:A:271:PRO:HA	1:A:274:TYR:CE1	2.31	0.65
1:A:215:ASP:O	1:A:302:GLY:HA2	1.98	0.64
1:A:20:LEU:O	1:A:25:GLN:HB2	1.98	0.63
1:A:221:ILE:HD11	1:A:304:PRO:HG2	1.80	0.63
1:A:229:ASN:HA	1:A:232:VAL:CG1	2.25	0.63
1:A:303:ASP:HB3	1:A:307:ARG:NE	2.02	0.63
1:A:45:CYS:HA	1:A:105:THR:HA	1.81	0.63
1:A:229:ASN:CA	1:A:232:VAL:HG12	2.28	0.63
1:A:191:GLN:HB3	1:A:213:ILE:HG12	1.80	0.62
1:A:289:ILE:CG2	1:A:291:LEU:CD1	2.77	0.62
1:A:240:VAL:CB	1:A:244:LEU:HD13	2.30	0.62
1:A:112:TYR:C	1:A:112:TYR:CD2	2.78	0.61
1:A:248:THR:HG22	1:A:250:GLY:H	1.65	0.61
2:I:2:VAL:HG12	2:I:4:STA:CD2	2.29	0.61
1:A:147:GLU:HG3	1:A:148:GLN:N	2.15	0.61
1:A:14:SER:HB2	4:A:355:HOH:O	2.01	0.60
1:A:260:TYR:CE1	1:A:301:LEU:HD21	2.36	0.60
1:A:274:TYR:O	1:A:275:LEU:HD12	2.01	0.60
1:A:317:ASN:HB2	1:A:319:THR:OG1	2.01	0.60
1:A:125:TRP:HZ2	1:A:190:TRP:CZ3	2.20	0.60
1:A:268:THR:O	1:A:269:LEU:HD12	2.02	0.60
1:A:312:VAL:HB	1:A:321:GLY:HA3	1.85	0.59
1:A:135:PRO:HG2	1:A:138:VAL:CG2	2.27	0.59
1:A:247:THR:OG1	1:A:248:THR:N	2.35	0.59
1:A:221:ILE:CD1	1:A:304:PRO:HG2	2.33	0.59
1:A:199:PHE:CD2	1:A:227:PHE:HE1	2.21	0.59
1:A:89:VAL:HB	1:A:136:TYR:HE1	1.66	0.59
1:A:251:ASN:HB3	1:A:255:LEU:CD1	2.27	0.59
1:A:152:SER:HB2	1:A:310:PHE:HZ	1.68	0.58
1:A:37:ASN:HD22	1:A:38:VAL:N	2.01	0.58
1:A:107:ILE:HD12	1:A:107:ILE:N	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PRO:O	1:A:289:ILE:HG12	2.04	0.58
1:A:258:LEU:HB2	1:A:269:LEU:HB2	1.85	0.58
1:A:245:TYR:OH	1:A:287:VAL:HG23	2.03	0.57
1:A:223:VAL:CG1	1:A:227:PHE:HB3	2.34	0.57
1:A:83:ILE:O	1:A:103:GLU:HB2	2.04	0.57
2:I:3:VAL:O	2:I:4:STA:HG	2.04	0.57
1:A:216:SER:CB	1:A:306:MET:HE1	2.34	0.57
1:A:274:TYR:CD2	1:A:286:ILE:HD11	2.39	0.56
1:A:41:PRO:HA	1:A:104:MET:HE2	1.88	0.56
1:A:222:THR:HG22	1:A:223:VAL:N	2.21	0.56
1:A:72:LYS:HG2	1:A:74:THR:HG23	1.89	0.55
1:A:221:ILE:O	1:A:286:ILE:HA	2.07	0.55
1:A:268:THR:C	1:A:269:LEU:HD12	2.31	0.55
1:A:223:VAL:HG12	1:A:227:PHE:HB3	1.89	0.55
1:A:324:LEU:HG	1:A:325:ALA:N	2.11	0.55
1:A:223:VAL:HG12	1:A:224:PRO:O	2.07	0.54
1:A:199:PHE:CD2	1:A:227:PHE:CE1	2.95	0.54
1:A:7:LYS:CG	1:A:15:PHE:HE2	2.20	0.54
1:A:183:LYS:NZ	1:A:319:THR:HG23	2.22	0.54
1:A:148:GLN:HG2	1:A:316:ASP:OD2	2.08	0.54
1:A:193:ASP:O	1:A:194:LEU:HD23	2.06	0.54
1:A:220:VAL:HG22	1:A:285:ASN:CA	2.37	0.54
1:A:224:PRO:HD3	1:A:298:THR:O	2.08	0.54
1:A:303:ASP:N	1:A:304:PRO:CD	2.68	0.54
1:A:89:VAL:HG23	1:A:99:TYR:HB3	1.89	0.53
1:A:222:THR:CG2	1:A:223:VAL:N	2.72	0.53
1:A:228:PHE:CD1	1:A:288:PRO:HB3	2.42	0.53
1:A:243:LEU:O	1:A:244:LEU:HD12	2.08	0.53
1:A:172:GLU:HA	1:A:175:PHE:CE2	2.43	0.53
1:A:125:TRP:CZ2	1:A:190:TRP:CH2	2.97	0.53
1:A:312:VAL:O	1:A:321:GLY:N	2.19	0.53
1:A:191:GLN:HE21	1:A:211:ASN:HD21	1.55	0.53
1:A:151:TYR:CD1	1:A:313:TYR:HB2	2.44	0.52
1:A:198:HIS:CD2	1:A:206:SER:HB3	2.44	0.52
1:A:239:LYS:NZ	1:A:245:TYR:HE1	1.95	0.52
1:A:173:ARG:O	1:A:326:LYS:HG3	2.10	0.52
1:A:13:LEU:HB2	1:A:307:ARG:HH12	1.74	0.52
1:A:15:PHE:HA	1:A:29:PHE:O	2.10	0.52
1:A:222:THR:HB	1:A:300:VAL:HB	1.90	0.52
1:A:78:GLY:HA3	1:A:109:GLY:CA	2.39	0.52
1:A:27:PHE:HB2	1:A:29:PHE:HE1	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLY:C	1:A:304:PRO:HD2	2.36	0.51
1:A:312:VAL:HG12	1:A:313:TYR:N	2.24	0.51
1:A:125:TRP:HZ2	1:A:190:TRP:CH2	2.28	0.51
1:A:147:GLU:CG	1:A:148:GLN:H	2.23	0.51
1:A:264:ASN:N	1:A:264:ASN:ND2	2.58	0.51
1:A:9:LEU:HD21	1:A:116:ASP:HB2	1.93	0.51
1:A:4:VAL:HG12	1:A:165:LEU:HB3	1.93	0.51
1:A:38:VAL:HG23	1:A:121:PHE:HA	1.92	0.51
1:A:112:TYR:C	1:A:112:TYR:HD2	2.18	0.50
1:A:310:PHE:CE2	1:A:312:VAL:HG22	2.46	0.50
1:A:19:LYS:HB2	1:A:90:THR:HB	1.93	0.50
1:A:127:ASP:OD1	4:A:365:HOH:O	2.20	0.50
1:A:110:PRO:HD2	1:A:111:PHE:CD2	2.46	0.50
1:A:62:LYS:HB2	1:A:62:LYS:HZ2	1.77	0.50
1:A:258:LEU:N	1:A:269:LEU:O	2.41	0.49
1:A:185:ASN:HD22	1:A:192:VAL:HA	1.77	0.49
1:A:291:LEU:HD12	1:A:291:LEU:N	2.28	0.49
1:A:34:ALA:O	1:A:128:LEU:HD21	2.13	0.49
1:A:109(B):GLU:OE1	1:A:113:SER:HB3	2.12	0.49
1:A:126:LYS:O	1:A:129:SER:HB3	2.12	0.49
1:A:256:PRO:O	1:A:274:TYR:OH	2.29	0.49
1:A:191:GLN:HE21	1:A:211:ASN:ND2	2.10	0.49
1:A:220:VAL:CG1	1:A:287:VAL:HG12	2.41	0.48
1:A:278:LEU:HD21	1:A:283:MET:HG3	1.94	0.48
1:A:20:LEU:HB2	1:A:27:PHE:HE1	1.78	0.48
1:A:258:LEU:O	1:A:268:THR:HA	2.13	0.48
1:A:220:VAL:HG22	1:A:285:ASN:HA	1.95	0.48
1:A:243:LEU:C	1:A:244:LEU:HD12	2.38	0.48
1:A:185:ASN:HD21	1:A:211:ASN:ND2	2.12	0.48
1:A:296:LYS:O	1:A:297:ASN:C	2.56	0.48
1:A:17:GLU:OE2	1:A:26:LYS:CD	2.60	0.47
1:A:245:TYR:CD2	1:A:245:TYR:N	2.82	0.47
1:A:277:PRO:HA	1:A:282:CYS:SG	2.55	0.47
1:A:288:PRO:O	1:A:289:ILE:CG1	2.63	0.47
1:A:65:GLU:CB	1:A:86:LYS:HB3	2.45	0.47
1:A:260:TYR:CZ	1:A:301:LEU:HD21	2.50	0.47
1:A:299:PHE:CD1	1:A:299:PHE:N	2.82	0.47
1:A:21:GLY:O	1:A:88:LEU:HD23	2.14	0.46
1:A:151:TYR:CE1	1:A:313:TYR:CB	2.96	0.46
1:A:218:THR:O	1:A:302:GLY:HA3	2.16	0.46
1:A:218:THR:HG23	2:I:3:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:IVA:O	2:I:2:VAL:C	2.58	0.46
1:A:183:LYS:HA	1:A:183:LYS:CE	2.29	0.46
1:A:228:PHE:CG	1:A:288:PRO:HB3	2.51	0.46
1:A:151:TYR:OH	1:A:190:TRP:NE1	2.48	0.46
1:A:158:GLU:HB3	1:A:160:LYS:HD3	1.98	0.46
1:A:217:ALA:O	2:I:4:STA:HD22	2.16	0.45
1:A:39:TRP:NE1	1:A:120:VAL:HB	2.30	0.45
1:A:192:VAL:HG22	1:A:193:ASP:N	2.31	0.45
1:A:32:HIS:CD2	1:A:34:ALA:N	2.75	0.45
1:A:288:PRO:C	1:A:289:ILE:CG1	2.90	0.45
1:A:215:ASP:OD2	1:A:218:THR:OG1	2.34	0.45
1:A:240:VAL:HB	1:A:244:LEU:CD1	2.44	0.45
1:A:53:LYS:NZ	1:A:112:TYR:O	2.44	0.45
1:A:191:GLN:HB2	1:A:211:ASN:HD21	1.82	0.45
1:A:271:PRO:HA	1:A:274:TYR:CZ	2.52	0.44
1:A:220:VAL:HG13	1:A:285:ASN:C	2.41	0.44
1:A:257:THR:HG23	1:A:269:LEU:C	2.42	0.44
1:A:253:THR:C	1:A:255:LEU:H	2.26	0.44
1:A:111:PHE:HA	1:A:114:GLU:CD	2.42	0.44
1:A:284:LEU:HD12	1:A:284:LEU:N	2.26	0.44
1:A:235:ALA:O	1:A:236:SER:C	2.60	0.44
1:A:305:PHE:CD2	1:A:305:PHE:C	2.96	0.44
1:A:312:VAL:CB	1:A:321:GLY:HA3	2.48	0.43
1:A:6:LEU:HA	1:A:15:PHE:O	2.18	0.43
1:A:305:PHE:CE2	1:A:309:TYR:HB2	2.53	0.43
1:A:135:PRO:O	1:A:138:VAL:N	2.51	0.43
1:A:225:THR:O	1:A:229:ASN:ND2	2.50	0.43
1:A:314:ASP:OD2	1:A:317:ASN:CB	2.62	0.43
1:A:25:GLN:NE2	1:A:61:SER:HB2	2.34	0.43
1:A:198:HIS:O	1:A:199:PHE:CD1	2.72	0.43
1:A:109(B):GLU:HB3	1:A:110:PRO:HA	2.01	0.43
1:A:73:LEU:N	1:A:80:ILE:O	2.52	0.43
1:A:31:PHE:HB2	4:A:355:HOH:O	2.18	0.43
1:A:157:PRO:HG3	1:A:325:ALA:HB3	2.00	0.43
1:A:243(A):SER:HB2	1:A:245:TYR:OH	2.20	0.42
1:A:8:ASP:CA	1:A:13:LEU:HG	2.50	0.42
1:A:292:GLU:CG	1:A:296:LYS:H	2.28	0.42
1:A:136:TYR:CD2	1:A:140:LEU:HD11	2.54	0.42
1:A:19:LYS:HA	1:A:25:GLN:O	2.19	0.42
1:A:112:TYR:CD2	1:A:112:TYR:O	2.73	0.42
1:A:124:GLY:C	1:A:125:TRP:CD1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:HG2	2:I:6:STA:HB2	2.00	0.42
1:A:192:VAL:CG2	1:A:193:ASP:N	2.82	0.42
1:A:237:VAL:HG12	1:A:238:PHE:N	2.34	0.42
1:A:255:LEU:HA	1:A:255:LEU:HD23	1.83	0.42
1:A:10:ALA:O	1:A:11:ASN:C	2.62	0.42
1:A:27:PHE:CE2	1:A:40:VAL:HG11	2.55	0.42
1:A:21:GLY:HA3	1:A:61:SER:OG	2.19	0.41
1:A:62:LYS:HB2	1:A:62:LYS:HZ3	1.83	0.41
1:A:183:LYS:HZ1	1:A:319:THR:HG23	1.85	0.41
1:A:240:VAL:HG12	1:A:243:LEU:HB2	2.02	0.41
1:A:304:PRO:HA	1:A:307:ARG:HD2	2.02	0.41
1:A:107:ILE:N	1:A:107:ILE:CD1	2.81	0.41
1:A:228:PHE:HD2	1:A:232:VAL:HG11	1.86	0.41
1:A:65:GLU:HB2	1:A:86:LYS:HB3	2.01	0.41
1:A:15:PHE:CD2	1:A:15:PHE:C	2.98	0.41
1:A:96:VAL:CG2	1:A:98:PRO:HD2	2.50	0.41
1:A:289:ILE:CG2	1:A:291:LEU:HD11	2.49	0.41
1:A:310:PHE:N	1:A:323:ALA:O	2.53	0.41
1:A:159:ASN:C	1:A:159:ASN:HD22	2.29	0.40
1:A:266:VAL:HG13	1:A:268:THR:HG23	2.02	0.40
1:A:239:LYS:HE3	1:A:244:LEU:H	1.86	0.40
1:A:57:ASP:OD1	1:A:59:SER:OG	2.39	0.40

All (3) 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:A:126:LYS:NZ	1:A:162:LYS:NZ[4_455]	0.97	1.23
1:A:126:LYS:NZ	1:A:162:LYS:CE[4_455]	1.85	0.35
1:A:126:LYS:CE	1:A:162:LYS:NZ[4_455]	1.93	0.27

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	321/332 (97%)	276 (86%)	42 (13%)	3 (1%)	14	43
2	I	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
All	All	324/338 (96%)	278 (86%)	42 (13%)	4 (1%)	10	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	2	VAL
1	A	235	ALA
1	A	292	GLU
1	A	64	TYR

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	293/301 (97%)	242 (83%)	51 (17%)	2	9
2	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	295/303 (97%)	243 (82%)	52 (18%)	2	9

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	ASN
1	A	4	VAL
1	A	5	GLU
1	A	9	LEU
1	A	12	VAL
1	A	13	LEU
1	A	15	PHE
1	A	37	ASN
1	A	44	LYS

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Mol	Chain	Res	Type
1	A	62	LYS
1	A	63	THR
1	A	65	GLU
1	A	66	LYS
1	A	68	ASP
1	A	71	VAL
1	A	73	LEU
1	A	76	LYS
1	A	80	ILE
1	A	83	ILE
1	A	88	LEU
1	A	106	GLU
1	A	107	ILE
1	A	133	ILE
1	A	146	ILE
1	A	148	GLN
1	A	158	GLU
1	A	159	ASN
1	A	166	THR
1	A	171	GLU
1	A	183	LYS
1	A	186	HIS
1	A	220	VAL
1	A	224	PRO
1	A	225	THR
1	A	232	VAL
1	A	234	SER
1	A	242	PHE
1	A	245	TYR
1	A	246	VAL
1	A	248	THR
1	A	251	ASN
1	A	261	ARG
1	A	264	ASN
1	A	272	LYS
1	A	281	LEU
1	A	283	MET
1	A	303	ASP
1	A	311	THR
1	A	318	HIS
1	A	320	VAL
2	I	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	32	HIS
1	A	37	ASN
1	A	148	GLN
1	A	159	ASN
1	A	185	ASN
1	A	191	GLN
1	A	211	ASN
1	A	230	GLN
1	A	297	ASN
1	A	318	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	STA	I	4	2	10,10,11	1.16	1 (10%)	9,12,14	2.00	1 (11%)
2	STA	I	6	2	11,11,11	1.72	2 (18%)	11,14,14	1.38	1 (9%)

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	STA	I	4	2	-	4/11/11/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STA	I	6	2	-	10/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	6	STA	CB-CA	3.76	1.59	1.53
2	I	6	STA	CH-CA	2.62	1.55	1.53
2	I	4	STA	CM-C	2.09	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	STA	CM-CH-CA	5.14	120.86	112.93
2	I	6	STA	CH-CM-C	-3.55	106.10	113.93

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	4	STA	CA-CH-CM-C
2	I	6	STA	N-CA-CB-CG
2	I	6	STA	N-CA-CH-OH
2	I	6	STA	CA-CH-CM-C
2	I	6	STA	CA-CB-CG-CD2
2	I	6	STA	CA-CB-CG-CD1
2	I	4	STA	CA-CB-CG-CD1
2	I	4	STA	CA-CB-CG-CD2
2	I	6	STA	CB-CA-CH-OH
2	I	6	STA	N-CA-CH-CM
2	I	4	STA	OH-CH-CM-C
2	I	6	STA	CH-CA-CB-CG
2	I	6	STA	OH-CH-CM-C
2	I	6	STA	CB-CA-CH-CM

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	STA	4	0
2	I	6	STA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	502	-	3,3,3	0.38	0	2,2,2	0.80	0
3	EDO	A	501	-	3,3,3	0.74	0	2,2,2	0.15	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
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	A	501	EDO	O1-C1-C2-O2

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	323/332 (97%)	-0.24	7 (2%) 62 43	46, 65, 85, 94	1 (0%)
2	I	3/6 (50%)	0.27	1 (33%) 1 1	32, 32, 33, 61	3 (100%)
All	All	326/338 (96%)	-0.24	8 (2%) 58 39	32, 65, 85, 94	4 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	PRO	4.3
1	A	159	ASN	3.4
1	A	11	ASN	2.9
1	A	128	LEU	2.4
1	A	14	SER	2.4
1	A	155	LEU	2.2
2	I	5	ALA	2.0
1	A	279(A)	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å ²)	Q<0.9
2	STA	I	6	12/12	0.82	0.16	95,99,100,100	12
2	STA	I	4	11/12	0.92	0.10	40,49,72,74	11

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	501	4/4	0.82	0.11	59,59,61,61	0
3	EDO	A	502	4/4	0.83	0.07	70,71,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.