



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 4DOU / pdb_00004dou
Title : Crystal Structure of a Single-chain Trimer of Human Adiponectin Globular Domain
Authors : Min, X.; Walker, N.P.; Wang, Z.
Deposited on : 2012-02-10
Resolution : 2.00 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

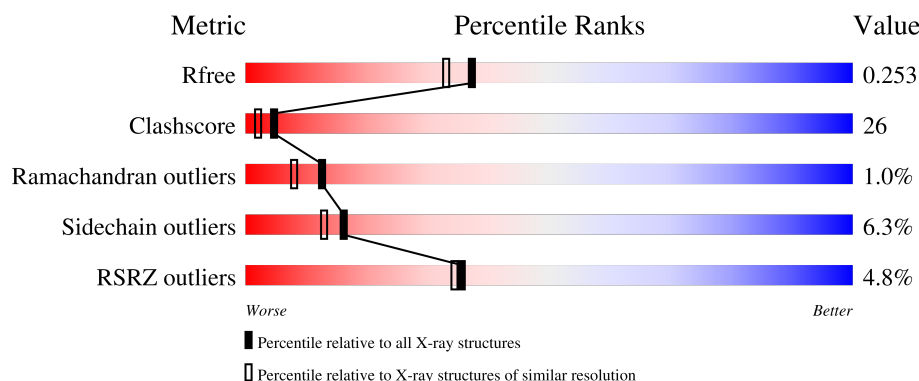
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	442	

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
4	GOL	A	1005	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1007	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3486 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 Adiponectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	3	0
			3298	2133	528	625	12			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	HIS	-	expression tag	UNP Q15848
A	88	HIS	-	expression tag	UNP Q15848
A	89	HIS	-	expression tag	UNP Q15848
A	90	HIS	-	expression tag	UNP Q15848
A	91	HIS	-	expression tag	UNP Q15848
A	92	HIS	-	expression tag	UNP Q15848
A	93	HIS	-	expression tag	UNP Q15848
A	94	HIS	-	expression tag	UNP Q15848
A	95	GLU	-	expression tag	UNP Q15848
A	96	ASN	-	expression tag	UNP Q15848
A	97	LEU	-	expression tag	UNP Q15848
A	98	TYR	-	expression tag	UNP Q15848
A	99	PHE	-	expression tag	UNP Q15848
A	100	GLN	-	expression tag	UNP Q15848
A	101	GLY	-	expression tag	UNP Q15848
A	102	ALA	-	expression tag	UNP Q15848
A	103	SER	-	expression tag	UNP Q15848

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	158	Total	O	0	0
			158	158		

i

- Molecule 1: Adiponectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.31Å 49.63Å 50.46Å 117.23° 101.68° 105.31°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.00) 91.0 (30.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.200 , 0.257 0.203 , 0.253	Depositor DCC
R_{free} test set	1166 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3486	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GOL, NA, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/3399	0.76	4/4605 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	ILE	CA-C-N	6.03	126.34	119.83
1	A	407	ILE	C-N-CA	6.03	126.34	119.83
1	A	120	GLU	N-CA-C	-6.02	105.75	114.12
1	A	297	GLY	N-CA-C	5.02	118.31	110.88

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	3298	0	3080	165	1
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	6	0
5	A	20	0	30	8	0
6	A	158	0	0	19	1
All	All	3486	0	3118	166	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (166) 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:500:GLU:HB2	1:A:502[A]:GLU:OE2	1.07	1.21
1:A:500:GLU:CB	1:A:502[A]:GLU:OE2	1.88	1.21
1:A:319:LYS:HE2	1:A:350:ASP:CB	1.78	1.12
1:A:319:LYS:HE2	1:A:350:ASP:HB3	1.14	1.11
1:A:243:THR:HG23	1:A:253:ARG:HH22	0.91	1.05
1:A:244:ASN:O	1:A:246:GLY:HA2	1.55	1.05
1:A:124:THR:HG22	1:A:222:ASN:HD22	1.19	1.05
1:A:431:LYS:NZ	4:A:1005:GOL:H2	1.75	1.02
1:A:243:THR:HG23	1:A:253:ARG:NH2	1.75	1.01
1:A:272:ARG:NH1	1:A:287:SER:HA	1.79	0.97
1:A:220:GLU:HA	6:A:1244:HOH:O	1.64	0.96
1:A:243:THR:CG2	1:A:253:ARG:HH22	1.78	0.96
1:A:319:LYS:HG2	1:A:350:ASP:HB2	1.50	0.93
1:A:385:ASN:HB2	1:A:386:PRO:HD3	1.52	0.90
1:A:124:THR:HG22	1:A:222:ASN:ND2	1.85	0.89
1:A:327:TYR:OH	1:A:329:GLN:HG3	1.73	0.89
1:A:455:VAL:HB	1:A:495:LEU:HD11	1.55	0.89
1:A:402:GLU:O	1:A:403:THR:HG23	1.71	0.89
1:A:243:THR:O	1:A:244:ASN:O	1.91	0.88
1:A:249:ALA:HB3	6:A:1248:HOH:O	1.74	0.86
1:A:455:VAL:HB	1:A:495:LEU:CD1	2.03	0.86
1:A:204:HIS:H	5:A:1007:EDO:H22	1.41	0.85
1:A:243:THR:HG21	6:A:1252:HOH:O	1.76	0.85
1:A:431:LYS:HZ2	4:A:1005:GOL:H2	1.41	0.83
1:A:359:GLU:N	6:A:1253:HOH:O	2.08	0.83
1:A:415:THR:O	1:A:417:ILE:CD1	2.27	0.82
1:A:472:GLN:OE1	6:A:1256:HOH:O	1.99	0.80
1:A:353:TRP:HE1	1:A:355:GLN:NE2	1.80	0.79
1:A:500:GLU:HB2	1:A:502[A]:GLU:CD	2.08	0.78
1:A:500:GLU:CA	1:A:502[A]:GLU:OE2	2.33	0.77
1:A:272:ARG:HH12	1:A:287:SER:HA	1.50	0.76
1:A:203:LEU:HA	5:A:1007:EDO:H22	1.69	0.75
1:A:431:LYS:HZ1	4:A:1005:GOL:H2	1.52	0.75
1:A:407:ILE:HD12	1:A:410:MET:HB2	1.68	0.74
1:A:224:LEU:H	1:A:224:LEU:HD12	1.54	0.72
1:A:204:HIS:H	5:A:1007:EDO:C2	2.04	0.70
1:A:455:VAL:CB	1:A:495:LEU:HD11	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:C	1:A:407:ILE:HD13	2.16	0.69
1:A:488:GLU:HB3	6:A:1151:HOH:O	1.93	0.69
1:A:170:ASP:OD2	1:A:221:ARG:NH1	2.26	0.68
1:A:272:ARG:NH1	1:A:286:GLY:O	2.26	0.68
1:A:327:TYR:CZ	1:A:329:GLN:HG3	2.31	0.66
1:A:204:HIS:N	5:A:1007:EDO:H22	2.12	0.63
1:A:163:HIS:C	1:A:164[A]:ILE:HD13	2.23	0.63
1:A:191:GLU:O	1:A:192:ASN:HB2	1.98	0.63
1:A:416:LYS:HE2	1:A:418:PHE:CE2	2.33	0.63
1:A:353:TRP:HE1	1:A:355:GLN:HE21	1.44	0.63
1:A:243:THR:O	1:A:244:ASN:C	2.41	0.62
1:A:177:LYS:HE2	1:A:178:LYS:HE2	1.82	0.62
1:A:341:SER:OG	1:A:445:HIS:HE1	1.83	0.61
1:A:149:LYS:HD3	1:A:210:GLN:NE2	2.15	0.61
1:A:204:HIS:HE1	1:A:206:GLU:OE1	1.84	0.61
1:A:404:TYR:HB2	6:A:1249:HOH:O	2.00	0.61
1:A:327:TYR:OH	1:A:329:GLN:CG	2.47	0.61
1:A:395:SER:OG	1:A:424:HIS:HD2	1.82	0.61
1:A:407:ILE:HD12	1:A:410:MET:CG	2.30	0.61
1:A:319:LYS:CG	1:A:350:ASP:HB2	2.27	0.61
1:A:296:PRO:HG3	1:A:348:VAL:HG23	1.83	0.60
1:A:272:ARG:NH1	1:A:287:SER:CA	2.61	0.59
1:A:407:ILE:O	1:A:407:ILE:HG23	2.03	0.59
1:A:244:ASN:O	1:A:246:GLY:CA	2.42	0.58
1:A:163:HIS:O	1:A:164[A]:ILE:HD13	2.03	0.58
1:A:415:THR:O	1:A:417:ILE:HD13	2.02	0.58
1:A:306:THR:CG2	1:A:372:ASP:O	2.52	0.58
1:A:500:GLU:C	1:A:502[A]:GLU:OE2	2.46	0.58
1:A:151:HIS:HE1	6:A:1118:HOH:O	1.85	0.58
1:A:167:TYR:O	1:A:168:MET:HB2	2.04	0.57
1:A:239:LEU:HD11	1:A:378:PHE:CG	2.40	0.57
1:A:243:THR:C	1:A:244:ASN:O	2.47	0.57
1:A:407:ILE:HD12	1:A:410:MET:CB	2.32	0.57
1:A:341:SER:OG	1:A:445:HIS:CE1	2.58	0.56
1:A:460:LYS:HG2	6:A:1212:HOH:O	2.05	0.56
1:A:168:MET:HE2	6:A:1170:HOH:O	2.04	0.56
1:A:243:THR:CG2	1:A:253:ARG:NH2	2.52	0.56
1:A:396:ALA:H	1:A:422:GLN:NE2	2.04	0.56
1:A:308:TYR:O	1:A:309:MET:HB3	2.05	0.56
1:A:318:LYS:HE3	1:A:346:LEU:HD23	1.87	0.56
1:A:407:ILE:HG23	1:A:410:MET:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:N	6:A:1216:HOH:O	2.40	0.55
1:A:319:LYS:CE	1:A:350:ASP:CB	2.69	0.54
1:A:416:LYS:C	1:A:417:ILE:HD12	2.32	0.54
1:A:415:THR:O	1:A:417:ILE:HD12	2.04	0.54
1:A:117:VAL:HG21	1:A:132:PHE:HB2	1.88	0.54
1:A:178:LYS:HB3	6:A:1105:HOH:O	2.08	0.54
1:A:416:LYS:HE2	1:A:418:PHE:CZ	2.44	0.53
1:A:117:VAL:CG2	1:A:132:PHE:HB2	2.39	0.53
1:A:318:LYS:O	1:A:319:LYS:HB2	2.09	0.53
1:A:117:VAL:HG23	1:A:132:PHE:CB	2.39	0.52
1:A:254:SER:OG	1:A:283:HIS:CD2	2.63	0.52
1:A:243:THR:O	1:A:243:THR:OG1	2.21	0.52
1:A:255:ALA:H	1:A:281:GLN:NE2	2.08	0.52
1:A:411:PRO:CD	4:A:1005:GOL:H12	2.40	0.51
1:A:332:GLU:HG2	1:A:333:ASN:OD1	2.09	0.51
1:A:417:ILE:HD12	1:A:417:ILE:N	2.25	0.51
1:A:306:THR:HG23	1:A:372:ASP:O	2.11	0.50
1:A:284:TYR:CE2	1:A:286:GLY:HA2	2.46	0.50
1:A:402:GLU:O	1:A:403:THR:CG2	2.54	0.50
1:A:177:LYS:HG2	1:A:178:LYS:HG2	1.93	0.50
1:A:385:ASN:HB2	1:A:386:PRO:CD	2.34	0.50
1:A:502[A]:GLU:CD	1:A:502[A]:GLU:H	2.18	0.50
1:A:117:VAL:CG2	1:A:132:PHE:CB	2.90	0.50
1:A:175:LEU:HD23	1:A:213:LEU:HD23	1.93	0.50
1:A:449:TYR:O	1:A:450:MET:HB2	2.11	0.50
1:A:407:ILE:HD13	1:A:408:PRO:N	2.27	0.49
1:A:220:GLU:CG	1:A:221:ARG:N	2.74	0.49
1:A:305:ILE:HD12	1:A:365:LEU:HD23	1.94	0.49
1:A:407:ILE:C	1:A:407:ILE:CD1	2.84	0.49
1:A:407:ILE:HD12	1:A:410:MET:HG3	1.95	0.49
1:A:385:ASN:CB	1:A:386:PRO:HD3	2.32	0.49
1:A:343:LEU:HB2	1:A:398:SER:HB2	1.95	0.48
1:A:455:VAL:CG2	1:A:495:LEU:HD11	2.43	0.48
1:A:459:LYS:HE3	1:A:487:LEU:HD23	1.95	0.48
1:A:499:GLY:HA3	6:A:1234:HOH:O	2.13	0.48
1:A:116:SER:HB2	1:A:484:LEU:HB2	1.94	0.48
1:A:210:GLN:NE2	6:A:1169:HOH:O	2.46	0.48
1:A:306:THR:HG21	6:A:1150:HOH:O	2.14	0.48
1:A:269:MET:HE3	1:A:270:PRO:HD2	1.96	0.48
1:A:296:PRO:HG3	1:A:348:VAL:CG2	2.42	0.47
1:A:215:VAL:HG11	1:A:220:GLU:OE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:HIS:ND1	5:A:1006:EDO:H21	2.30	0.46
1:A:280:GLN:O	1:A:280:GLN:HG3	2.14	0.46
1:A:254:SER:OG	1:A:283:HIS:HD2	1.97	0.46
1:A:424:HIS:HE1	6:A:1198:HOH:O	1.99	0.46
1:A:297:GLY:HA2	1:A:383:ASP:OD1	2.16	0.46
1:A:220:GLU:HG3	1:A:221:ARG:H	1.82	0.45
1:A:224:LEU:H	1:A:224:LEU:CD1	2.27	0.45
1:A:128:MET:O	1:A:214:GLN:HB2	2.16	0.45
1:A:203:LEU:CA	5:A:1007:EDO:H22	2.43	0.45
1:A:159:TYR:O	1:A:236:GLY:HA2	2.17	0.45
1:A:215:VAL:CG1	1:A:220:GLU:OE2	2.65	0.45
1:A:224:LEU:HD12	1:A:224:LEU:N	2.26	0.45
1:A:411:PRO:HG2	4:A:1005:GOL:H12	1.99	0.44
1:A:204:HIS:O	5:A:1007:EDO:H11	2.17	0.44
1:A:419:TYR:CZ	1:A:421:GLN:CB	3.01	0.44
1:A:353:TRP:NE1	1:A:355:GLN:HE21	2.14	0.44
1:A:284:TYR:HE2	1:A:286:GLY:HA2	1.82	0.43
1:A:411:PRO:CG	4:A:1005:GOL:H12	2.47	0.43
1:A:124:THR:O	1:A:124:THR:OG1	2.36	0.43
1:A:169:LYS:O	1:A:223:GLY:HA3	2.18	0.43
1:A:385:ASN:CB	1:A:386:PRO:CD	2.97	0.43
1:A:403:THR:HB	1:A:404:TYR:H	1.55	0.42
1:A:183:LEU:HD23	1:A:184:PHE:N	2.35	0.42
1:A:269:MET:HE3	1:A:269:MET:HB3	1.83	0.42
1:A:166:VAL:HG13	1:A:171:VAL:CG1	2.50	0.42
1:A:419:TYR:CZ	1:A:421:GLN:HB2	2.55	0.42
1:A:300:TYR:O	1:A:377:GLY:HA2	2.19	0.42
1:A:399:VAL:CG2	1:A:414:PHE:HB2	2.49	0.42
1:A:417:ILE:CD1	1:A:417:ILE:N	2.83	0.42
5:A:1006:EDO:H11	6:A:1251:HOH:O	2.19	0.42
1:A:244:ASN:C	1:A:246:GLY:HA2	2.37	0.41
1:A:183:LEU:CD2	1:A:184:PHE:N	2.83	0.41
1:A:111:TYR:HD2	6:A:1181:HOH:O	2.03	0.41
1:A:369:ASN:HB2	6:A:1156:HOH:O	2.21	0.41
1:A:301:PHE:O	1:A:341:SER:HA	2.20	0.41
1:A:408:PRO:O	1:A:409:ASN:HB2	2.19	0.41
1:A:451:LYS:O	1:A:505:GLY:HA3	2.20	0.41
1:A:395:SER:OG	1:A:424:HIS:CD2	2.68	0.41
1:A:407:ILE:O	1:A:407:ILE:CG2	2.69	0.41
1:A:432:PHE:O	1:A:492:GLN:HA	2.20	0.41
1:A:317:PHE:O	1:A:352:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HE2	1:A:178:LYS:CE	2.49	0.40
1:A:220:GLU:CG	1:A:221:ARG:H	2.35	0.40
1:A:325:PHE:HE2	1:A:357:TYR:CZ	2.39	0.40
1:A:455:VAL:HB	1:A:495:LEU:HD13	1.93	0.40
1:A:183:LEU:HD23	1:A:184:PHE:H	1.85	0.40
1:A:244:ASN:HB3	1:A:245:PRO:CD	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:OE1	6:A:1190:HOH:O[1_666]	1.73	0.47

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	390/442 (88%)	354 (91%)	32 (8%)	4 (1%)	12 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	403	THR
1	A	138	ASN
1	A	385	ASN

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	354/385 (92%)	332 (94%)	22 (6%)	16	13

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	TYR
1	A	141	ASN
1	A	157	LEU
1	A	171	VAL
1	A	175	LEU
1	A	183	LEU
1	A	213	LEU
1	A	221	ARG
1	A	239	LEU
1	A	243	THR
1	A	298	LEU
1	A	306	THR
1	A	351	GLN
1	A	380	LEU
1	A	403	THR
1	A	407	ILE
1	A	439	LEU
1	A	457	LEU
1	A	460	LYS
1	A	473	GLU
1	A	495	LEU
1	A	521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	140	GLN
1	A	151	HIS
1	A	192	ASN
1	A	196	GLN
1	A	204	HIS
1	A	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	GLN
1	A	283	HIS
1	A	292	HIS
1	A	337	GLN
1	A	351	GLN
1	A	355	GLN
1	A	422	GLN
1	A	424	HIS
1	A	445	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
4	GOL	A	1005	-	5,5,5	0.32	0	5,5,5	0.27	0
5	EDO	A	1008	-	3,3,3	0.42	0	2,2,2	0.40	0
5	EDO	A	1006	-	3,3,3	0.35	0	2,2,2	0.49	0
5	EDO	A	1010	-	3,3,3	0.43	0	2,2,2	0.42	0
5	EDO	A	1007	-	3,3,3	0.44	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1009	-	3,3,3	0.42	0	2,2,2	0.40	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
4	GOL	A	1005	-	-	0/4/4/4	-
5	EDO	A	1008	-	-	1/1/1/1	-
5	EDO	A	1006	-	-	1/1/1/1	-
5	EDO	A	1010	-	-	1/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	A	1009	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1006	EDO	O1-C1-C2-O2
5	A	1009	EDO	O1-C1-C2-O2
5	A	1007	EDO	O1-C1-C2-O2
5	A	1010	EDO	O1-C1-C2-O2
5	A	1008	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	GOL	6	0
5	A	1006	EDO	2	0
5	A	1007	EDO	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	399/442 (90%)	0.16	19 (4%) 35 34	13, 30, 50, 67	3 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	GLU	3.5
1	A	124	THR	3.5
1	A	386	PRO	3.3
1	A	403	THR	3.3
1	A	357	TYR	3.2
1	A	461	ASP	3.1
1	A	245	PRO	2.9
1	A	123	VAL	2.8
1	A	122	TYR	2.7
1	A	216	TYR	2.6
1	A	404	TYR	2.6
1	A	407	ILE	2.5
1	A	248	GLY	2.3
1	A	525	THR	2.3
1	A	244	ASN	2.3
1	A	500	GLU	2.1
1	A	246	GLY	2.1
1	A	243	THR	2.1
1	A	472	GLN	2.0

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

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

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
5	EDO	A	1008	4/4	0.70	0.14	47,47,48,48	0
5	EDO	A	1007	4/4	0.83	0.17	35,35,35,37	0
5	EDO	A	1010	4/4	0.84	0.12	43,43,43,43	0
5	EDO	A	1006	4/4	0.87	0.22	32,34,34,35	0
4	GOL	A	1005	6/6	0.87	0.10	41,41,41,42	0
5	EDO	A	1009	4/4	0.88	0.11	40,41,42,43	0
2	CA	A	1002	1/1	0.98	0.03	25,25,25,25	0
3	NA	A	1004	1/1	0.98	0.04	30,30,30,30	0
2	CA	A	1003	1/1	0.99	0.03	27,27,27,27	0
2	CA	A	1001	1/1	0.99	0.03	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.