



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:46 PM UTC

PDB ID : 7CI1 / pdb_00007ci1
Title : Crystal structure of AcrVA2
Authors : Chen, P.; Cheng, Z.; Wang, Y.
Deposited on : 2020-07-07
Resolution : 2.30 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

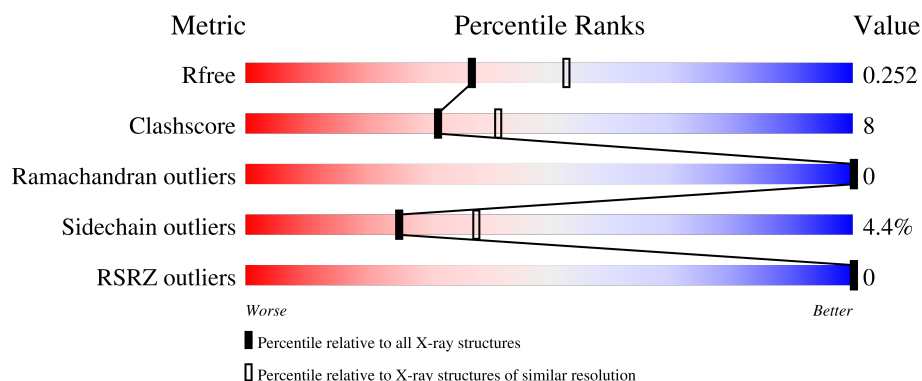
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	323	
1	B	323	

2 Entry composition [i](#)

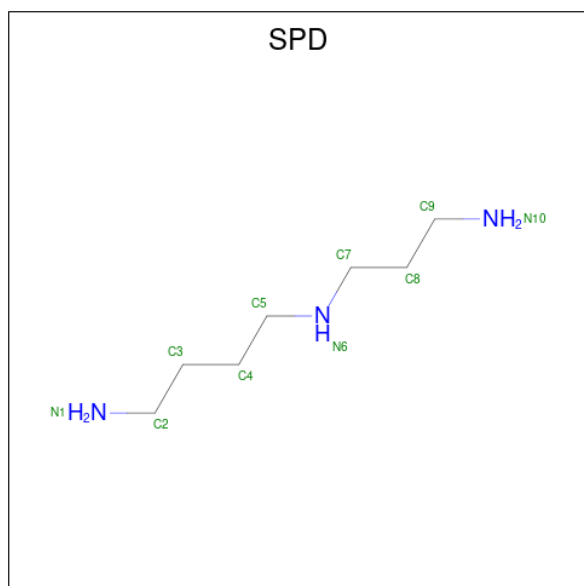
There are 4 unique types of molecules in this entry. The entry contains 4879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AcrVA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2342	1511	398	425	8			
1	B	295	Total	C	N	O	S	0	2	0
			2336	1508	397	422	9			

- Molecule 2 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		
2	A	1	Total	C	N	0	0
			10	7	3		
2	B	1	Total	C	N	0	0
			10	7	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

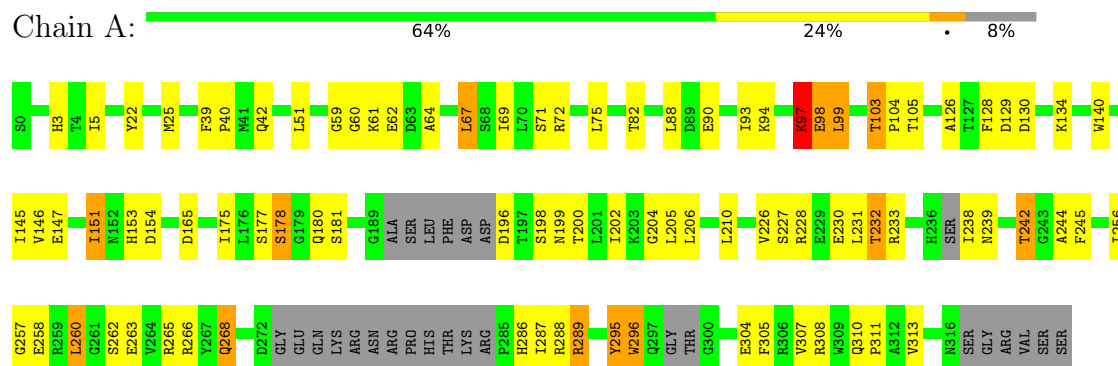
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 70 70	0	0
4	B	65	Total O 65 65	0	0

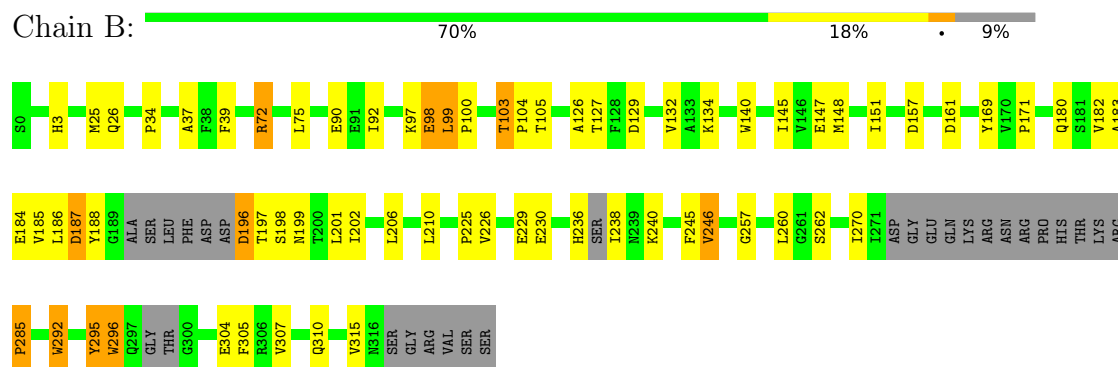
3 Residue-property plots [i](#)

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: AcrVA2



• Molecule 1: AcrVA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	84.29Å 84.29Å 264.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.97 – 2.30 48.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (48.97-2.30) 86.3 (48.97-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.229 , 0.251 0.230 , 0.252	Depositor DCC
R_{free} test set	2003 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4879	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: EDO, SPD

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	1.34	26/2408 (1.1%)	1.15	22/3276 (0.7%)
1	B	1.05	19/2406 (0.8%)	1.02	18/3275 (0.5%)
All	All	1.20	45/4814 (0.9%)	1.09	40/6551 (0.6%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	LEU	C-O	-9.27	1.15	1.24
1	B	292	TRP	C-N	-7.70	1.23	1.33
1	B	98	GLU	CA-C	-7.66	1.43	1.52
1	A	134	LYS	C-O	-6.71	1.15	1.23
1	A	175	ILE	C-O	-6.71	1.16	1.24
1	A	98	GLU	CA-C	-6.60	1.44	1.52
1	A	287	ILE	C-O	-6.35	1.17	1.24
1	A	97	LYS	CA-C	-6.20	1.45	1.52
1	A	265[A]	ARG	CA-C	6.16	1.61	1.52
1	A	265[B]	ARG	CA-C	6.16	1.61	1.52
1	A	258	GLU	C-O	-6.12	1.16	1.24
1	B	226	VAL	C-O	-5.96	1.17	1.24
1	A	226	VAL	C-O	-5.92	1.17	1.24
1	A	204	GLY	C-O	-5.91	1.16	1.23
1	B	225	PRO	C-O	-5.90	1.17	1.23
1	A	202	ILE	N-CA	-5.79	1.39	1.46
1	B	185	VAL	C-O	-5.75	1.17	1.24
1	A	181	SER	CA-C	-5.69	1.46	1.52
1	B	229	GLU	C-O	-5.64	1.17	1.24
1	A	71	SER	C-O	-5.63	1.17	1.24
1	B	246	VAL	C-O	-5.61	1.18	1.24
1	B	310	GLN	C-O	-5.58	1.17	1.24
1	B	105	THR	C-O	-5.53	1.17	1.24
1	A	260	LEU	C-O	-5.49	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	LEU	C-O	-5.44	1.17	1.24
1	A	310	GLN	C-O	-5.39	1.18	1.24
1	A	67	LEU	C-O	-5.35	1.17	1.24
1	A	205	LEU	C-O	-5.34	1.17	1.24
1	B	134	LYS	C-O	-5.32	1.17	1.23
1	A	200	THR	C-O	-5.31	1.18	1.24
1	A	105	THR	C-O	-5.26	1.17	1.24
1	B	169	TYR	C-O	-5.24	1.17	1.24
1	A	60	GLY	C-O	-5.22	1.17	1.23
1	B	188	TYR	CA-C	-5.22	1.48	1.52
1	B	97	LYS	C-O	-5.20	1.15	1.23
1	A	228	ARG	C-O	-5.20	1.18	1.24
1	B	201	LEU	C-O	-5.14	1.18	1.24
1	A	64	ALA	C-O	-5.14	1.18	1.24
1	B	97	LYS	CA-C	-5.13	1.46	1.52
1	A	311	PRO	C-O	-5.11	1.17	1.23
1	B	99	LEU	CA-C	-5.08	1.46	1.52
1	B	127	THR	C-O	-5.02	1.18	1.23
1	A	72	ARG	C-O	-5.01	1.18	1.24
1	A	231	LEU	C-O	-5.00	1.18	1.24
1	B	202	ILE	C-O	-5.00	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASP	N-CA-C	-14.38	87.26	109.25
1	B	129	ASP	N-CA-C	-14.07	85.75	108.41
1	A	178	SER	N-CA-C	11.86	124.21	111.28
1	B	188	TYR	N-CA-C	-11.73	93.86	111.34
1	A	265[A]	ARG	CA-C-O	11.48	132.72	120.55
1	A	265[B]	ARG	CA-C-O	11.48	132.72	120.55
1	A	94	LYS	CB-CG-CD	-8.82	91.02	111.30
1	A	103	THR	CA-C-N	8.36	128.29	119.85
1	A	103	THR	C-N-CA	8.36	128.29	119.85
1	B	270	ILE	CA-C-N	7.96	136.03	121.70
1	B	270	ILE	C-N-CA	7.96	136.03	121.70
1	B	100	PRO	N-CA-C	-7.38	99.67	111.03
1	A	265[A]	ARG	N-CA-C	7.25	119.18	111.28
1	A	265[B]	ARG	N-CA-C	7.25	119.18	111.28
1	A	296	TRP	N-CA-C	7.24	121.64	110.42
1	B	296	TRP	N-CA-C	7.19	121.56	110.42
1	B	187	ASP	N-CA-C	6.73	121.20	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	B	99	LEU	CA-C-N	6.44	126.78	119.83
1	B	99	LEU	C-N-CA	6.44	126.78	119.83
1	B	285	PRO	N-CA-CB	6.32	109.96	103.00
1	B	295	TYR	N-CA-C	6.22	116.78	108.38
1	A	295	TYR	N-CA-C	6.20	116.74	108.38
1	A	130	ASP	N-CA-C	5.94	118.98	110.24
1	B	197	THR	N-CA-C	-5.91	104.76	111.14
1	B	132	VAL	N-CA-C	5.76	115.95	108.35
1	B	103	THR	CA-C-N	5.69	125.59	119.85
1	B	103	THR	C-N-CA	5.69	125.59	119.85
1	A	59	GLY	CA-C-N	5.41	125.95	120.00
1	A	59	GLY	C-N-CA	5.41	125.95	120.00
1	A	128	PHE	N-CA-C	5.36	117.56	108.02
1	B	246	VAL	N-CA-CB	5.36	118.53	111.25
1	A	245	PHE	CA-C-N	-5.28	116.64	123.19
1	A	245	PHE	C-N-CA	-5.28	116.64	123.19
1	A	175	ILE	N-CA-C	5.25	115.87	109.30
1	A	99	LEU	CB-CA-C	-5.15	102.24	109.96
1	A	242	THR	N-CA-CB	-5.14	103.53	110.67
1	A	128	PHE	CB-CA-C	-5.09	102.93	110.62
1	B	230	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	286	HIS	N-CA-C	5.02	116.83	109.24

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	2342	0	2241	42	0
1	B	2336	0	2226	32	0
2	A	20	0	38	1	0
2	B	10	0	19	1	0
3	A	28	0	42	4	0
3	B	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	70	0	0	2	0
4	B	65	0	0	4	0
All	All	4879	0	4578	75	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 8.

All (75) 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:42:GLN:HE22	1:A:147:GLU:H	1.10	0.94
1:A:227:SER:OG	1:A:230:GLU:HG3	1.84	0.77
1:B:285:PRO:N	1:B:315:VAL:O	2.17	0.77
1:A:42:GLN:HE22	1:A:147:GLU:N	1.83	0.75
1:A:82:THR:HA	3:A:407:EDO:H22	1.71	0.73
2:A:401:SPD:N1	4:A:501:HOH:O	2.25	0.69
1:B:180:GLN:HB3	1:B:184:GLU:OE1	1.98	0.63
1:B:37:ALA:HB3	1:B:145:ILE:HD11	1.82	0.61
2:B:401:SPD:N10	4:B:503:HOH:O	2.31	0.61
1:A:288:ARG:HB3	1:A:313:VAL:CG2	2.30	0.61
1:B:296:TRP:CE3	1:B:304:GLU:O	2.54	0.60
1:A:151:ILE:HG23	1:A:153:HIS:CE1	2.37	0.60
1:A:296:TRP:CE3	1:A:304:GLU:O	2.54	0.60
1:A:90:GLU:O	1:A:93:ILE:HG22	2.02	0.59
1:A:88:LEU:HD23	1:A:256:ILE:HB	1.83	0.59
1:A:178:SER:HB3	1:A:180:GLN:HG3	1.84	0.59
1:A:268:GLN:HE21	1:A:268:GLN:CA	2.18	0.57
1:B:90:GLU:OE1	4:B:501:HOH:O	2.18	0.56
1:B:296:TRP:CH2	1:B:305:PHE:HD1	2.24	0.55
1:A:196:ASP:HA	1:A:199:ASN:HB2	1.88	0.55
1:A:22:TYR:HA	1:A:25:MET:HE3	1.87	0.55
1:A:296:TRP:CH2	1:A:305:PHE:HD1	2.24	0.55
1:B:296:TRP:CZ3	1:B:305:PHE:HD1	2.25	0.55
1:A:296:TRP:CZ3	1:A:305:PHE:HD1	2.25	0.54
1:A:296:TRP:HE3	1:A:304:GLU:O	1.90	0.54
1:B:296:TRP:HE3	1:B:304:GLU:O	1.90	0.54
1:B:196:ASP:HA	1:B:199:ASN:HB2	1.90	0.54
1:A:3:HIS:HD2	4:A:539:HOH:O	1.92	0.53
1:A:25:MET:HG2	1:A:39:PHE:CG	2.44	0.53
1:B:210:LEU:HD21	1:B:307:VAL:HG11	1.93	0.50
1:A:154:ASP:N	1:A:177:SER:OG	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:HB3	1:A:313:VAL:HG22	1.94	0.50
1:B:182:VAL:CG1	1:B:186:LEU:HD12	2.43	0.49
1:A:42:GLN:NE2	1:A:146:VAL:HA	2.27	0.49
1:B:3[A]:HIS:HE1	1:B:161:ASP:OD2	1.96	0.49
1:A:165:ASP:H	3:A:406:EDO:H11	1.77	0.48
1:A:230:GLU:HG2	1:A:233:ARG:NH2	2.29	0.48
1:A:296:TRP:CH2	1:A:305:PHE:CD1	3.02	0.48
1:B:3[B]:HIS:HD2	4:B:521:HOH:O	1.97	0.48
1:B:147:GLU:HG3	1:B:147:GLU:O	2.13	0.47
1:B:26:GLN:HB3	1:B:245:PHE:CE2	2.50	0.47
1:B:296:TRP:CH2	1:B:305:PHE:CD1	3.02	0.47
1:A:40:PRO:HB3	1:A:145:ILE:HG22	1.96	0.47
1:B:182:VAL:HG12	1:B:186:LEU:HD12	1.97	0.47
1:B:103:THR:HA	1:B:104:PRO:HD3	1.65	0.47
1:B:236:HIS:O	1:B:238:ILE:N	2.48	0.47
1:A:295:TYR:C	1:A:295:TYR:CD1	2.93	0.46
1:B:295:TYR:CD1	1:B:295:TYR:C	2.93	0.46
1:A:126:ALA:HB3	1:B:126:ALA:HB3	1.97	0.46
1:A:97:LYS:HD3	1:A:97:LYS:HA	1.61	0.45
1:B:37:ALA:HB3	1:B:145:ILE:CD1	2.46	0.45
1:A:238:ILE:HA	1:A:244:ALA:O	2.16	0.45
1:B:92:ILE:HG13	1:B:257:GLY:HA3	1.98	0.45
1:B:240:LYS:O	4:B:502:HOH:O	2.20	0.45
1:B:75:LEU:HD11	1:B:140:TRP:CG	2.52	0.45
1:A:75:LEU:HD11	1:A:140:TRP:CG	2.52	0.44
1:A:288:ARG:HB3	1:A:313:VAL:HG23	1.98	0.44
1:A:289:ARG:HA	1:A:289:ARG:HD2	1.80	0.44
1:B:140:TRP:CZ3	1:B:161:ASP:HB2	2.52	0.44
1:A:103:THR:HA	1:A:104:PRO:HD3	1.58	0.44
1:B:25:MET:HG2	1:B:39:PHE:CG	2.53	0.43
1:B:210:LEU:HD23	1:B:292:TRP:CD2	2.53	0.43
1:A:165:ASP:HB2	3:A:406:EDO:H11	2.01	0.43
1:A:5:ILE:CG2	3:A:405:EDO:H21	2.49	0.42
1:A:210:LEU:HD21	1:A:307:VAL:HG11	2.01	0.42
1:A:51:LEU:HD11	1:A:69:ILE:HG21	2.01	0.42
1:A:239:ASN:CG	1:A:242:THR:HB	2.45	0.41
1:B:34:PRO:HG2	1:B:37:ALA:O	2.20	0.41
1:B:99:LEU:HD11	1:B:206:LEU:HB3	2.02	0.41
1:A:257:GLY:HA2	1:A:260:LEU:HD12	2.02	0.41
1:A:232:THR:O	1:A:232:THR:CG2	2.69	0.40
1:B:157:ASP:HB3	1:B:171:PRO:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLN:HE21	1:A:268:GLN:C	2.29	0.40
1:A:263:GLU:O	1:A:266:ARG:HB3	2.20	0.40
1:B:183:ALA:O	1:B:187:ASP:HB2	2.21	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	287/323 (89%)	282 (98%)	5 (2%)	0	100	100
1	B	287/323 (89%)	283 (99%)	4 (1%)	0	100	100
All	All	574/646 (89%)	565 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	242/280 (86%)	229 (95%)	13 (5%)	20	29
1	B	241/280 (86%)	233 (97%)	8 (3%)	33	50
All	All	483/560 (86%)	462 (96%)	21 (4%)	25	39

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	62	GLU
1	A	67	LEU
1	A	97	LYS
1	A	98	GLU
1	A	99	LEU
1	A	151	ILE
1	A	198	SER
1	A	232	THR
1	A	262	SER
1	A	268	GLN
1	A	289	ARG
1	A	308	ARG
1	B	72	ARG
1	B	98	GLU
1	B	148	MET
1	B	151	ILE
1	B	196	ASP
1	B	198	SER
1	B	246	VAL
1	B	262	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	42	GLN
1	A	87	GLN
1	A	135	HIS
1	A	153	HIS
1	A	268	GLN
1	A	293	HIS
1	B	29	HIS
1	B	32	ASN
1	B	153	HIS
1	B	180	GLN
1	B	293	HIS

5.3.3 RNA ⓘ

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](#)

12 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	405	-	3,3,3	0.39	0	2,2,2	0.15	0
3	EDO	B	402	-	3,3,3	0.22	0	2,2,2	0.41	0
2	SPD	B	401	-	9,9,9	0.34	0	8,8,8	0.62	0
3	EDO	A	407	-	3,3,3	0.30	0	2,2,2	0.58	0
3	EDO	A	406	-	3,3,3	0.25	0	2,2,2	0.55	0
3	EDO	A	403	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	404	-	3,3,3	0.29	0	2,2,2	0.43	0
2	SPD	A	401	-	9,9,9	0.70	0	8,8,8	1.17	0
2	SPD	A	409	-	9,9,9	0.33	0	8,8,8	0.71	0
3	EDO	A	408	-	3,3,3	0.29	0	2,2,2	0.30	0
3	EDO	B	403	-	3,3,3	0.30	0	2,2,2	0.62	0
3	EDO	A	402	-	3,3,3	0.40	0	2,2,2	0.78	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	405	-	-	1/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
2	SPD	B	401	-	-	3/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	407	-	-	0/1/1/1	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-
2	SPD	A	401	-	-	3/7/7/7	-
2	SPD	A	409	-	-	3/7/7/7	-
3	EDO	A	408	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SPD	N6-C7-C8-C9
2	B	401	SPD	C8-C7-N6-C5
2	A	409	SPD	C8-C7-N6-C5
3	B	402	EDO	O1-C1-C2-O2
2	A	401	SPD	C7-C8-C9-N10
2	A	409	SPD	C7-C8-C9-N10
2	B	401	SPD	C7-C8-C9-N10
2	A	409	SPD	N1-C2-C3-C4
2	A	401	SPD	C2-C3-C4-C5
2	B	401	SPD	N1-C2-C3-C4
3	A	405	EDO	O1-C1-C2-O2
3	A	404	EDO	O1-C1-C2-O2
3	B	403	EDO	O1-C1-C2-O2
3	A	408	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	EDO	1	0
2	B	401	SPD	1	0
3	A	407	EDO	1	0
3	A	406	EDO	2	0
2	A	401	SPD	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 [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	296/323 (91%)	-1.17	0 100 100	8, 32, 71, 95	1 (0%)
1	B	295/323 (91%)	-1.16	0 100 100	7, 33, 73, 98	2 (0%)
All	All	591/646 (91%)	-1.17	0 100 100	7, 32, 73, 98	3 (0%)

There are no RSRZ outliers to report.

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 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(Å ²)	Q<0.9
3	EDO	A	403	4/4	0.97	0.09	35,36,48,50	0
3	EDO	A	404	4/4	0.98	0.09	34,39,41,54	0
3	EDO	A	405	4/4	0.98	0.07	35,37,37,41	0
3	EDO	B	402	4/4	0.98	0.06	36,37,40,44	0
3	EDO	B	403	4/4	0.98	0.06	35,38,45,48	0
2	SPD	A	409	10/10	0.99	0.05	24,33,37,37	0
2	SPD	B	401	10/10	0.99	0.05	20,33,38,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	406	4/4	0.99	0.06	42,43,48,49	0
3	EDO	A	407	4/4	0.99	0.07	32,35,35,42	0
3	EDO	A	408	4/4	0.99	0.06	37,37,40,42	0
3	EDO	A	402	4/4	0.99	0.05	30,35,36,42	0
2	SPD	A	401	10/10	0.99	0.04	20,24,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.