



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:25 PM UTC

PDB ID : 3AKO / pdb_00003ako
Title : Crystal Structure of the Reassembled Venus
Authors : Isogai, M.; Tada, T.
Deposited on : 2010-07-15
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

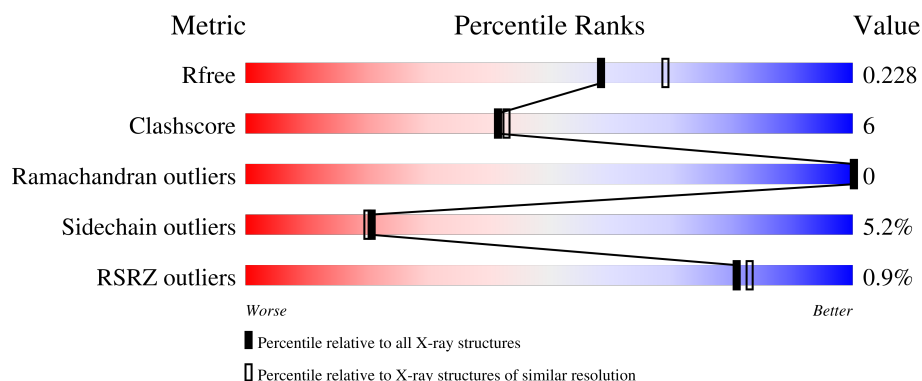
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	173	% 79% 9% • 12%
1	C	173	72% 11% • • 13%
1	E	173	% 69% 14% • 13%
1	G	173	% 72% 13% • • 13%
2	B	93	% 76% 8% • 14%

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Mol	Chain	Length	Quality of chain
2	D	93	72%10%18%
2	F	93	% 66%11%23%
2	H	93	2% 63%10%24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8022 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.

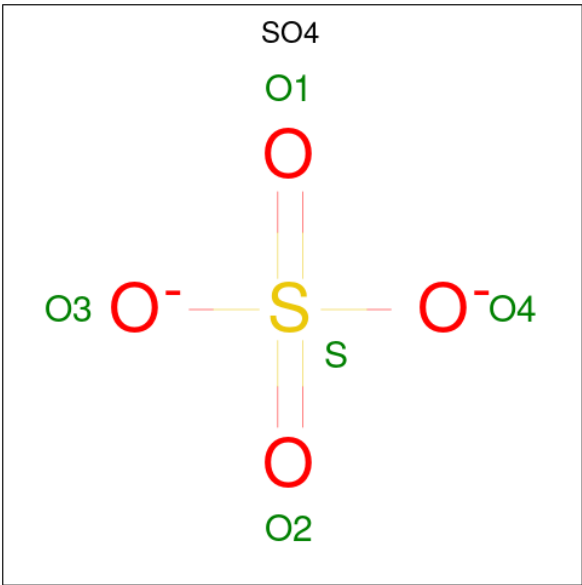
- Molecule 1 is a protein called Venus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	5	0
			1261	810	206	239	6			
1	C	150	Total	C	N	O	S	0	5	0
			1239	799	199	237	4			
1	E	150	Total	C	N	O	S	0	2	0
			1217	783	198	232	4			
1	G	150	Total	C	N	O	S	0	5	0
			1235	798	201	232	4			

- Molecule 2 is a protein called Venus.

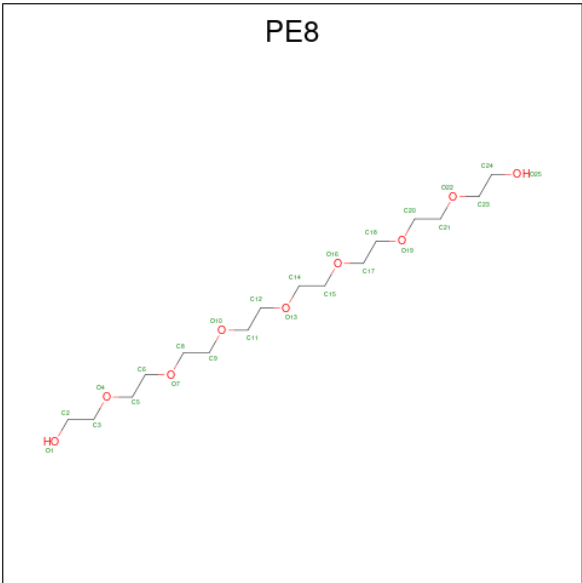
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	S	0	1	0
			632	396	112	122	2			
2	D	76	Total	C	N	O	S	0	1	0
			596	375	104	115	2			
2	F	72	Total	C	N	O	S	0	2	0
			579	363	106	109	1			
2	H	71	Total	C	N	O	S	0	4	0
			582	367	106	108	1			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			25	16	9		

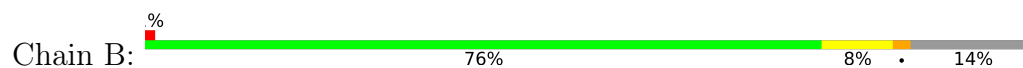
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total 135	O 135	0	0
5	B	60	Total 60	O 60	0	0
5	C	117	Total 117	O 117	0	0
5	D	62	Total 62	O 62	0	0
5	E	103	Total 103	O 103	0	0
5	F	39	Total 39	O 39	0	0
5	G	100	Total 100	O 100	0	0
5	H	35	Total 35	O 35	0	0

- Molecule 1: Venus



● Molecule 2: Venus



● Molecule 2: Venus



● Molecule 2: Venus



● Molecule 2: Venus



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.05Å 116.05Å 156.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 2.10 49.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.90-2.10) 99.9 (49.90-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.167 , 0.229 0.167 , 0.228	Depositor DCC
R_{free} test set	3228 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8022	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: CR2, PE8, SO4

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	0.91	0/1281	0.90	0/1725
1	C	0.91	1/1263 (0.1%)	0.92	0/1703
1	E	0.88	0/1231	0.95	0/1661
1	G	0.84	0/1258	0.93	1/1694 (0.1%)
2	B	0.93	0/647	0.96	2/873 (0.2%)
2	D	0.95	0/611	0.92	0/828
2	F	0.85	0/597	0.89	2/808 (0.2%)
2	H	0.81	0/606	0.96	0/820
All	All	0.89	1/7494 (0.0%)	0.93	5/10112 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	VAL	CA-CB	5.51	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	112	VAL	CB-CA-C	7.14	120.28	110.99
2	F	210	ASP	CA-C-N	5.83	125.50	119.56
2	F	210	ASP	C-N-CA	5.83	125.50	119.56
2	B	191	GLY	CA-C-N	5.06	124.99	119.78
2	B	191	GLY	C-N-CA	5.06	124.99	119.78

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	1261	0	1243	12	0
1	C	1239	0	1209	24	0
1	E	1217	0	1186	27	0
1	G	1235	0	1222	19	0
2	B	632	0	622	8	0
2	D	596	0	582	6	0
2	F	579	0	570	7	0
2	H	582	0	579	8	0
3	C	5	0	0	0	0
4	E	25	0	34	5	0
5	A	135	0	0	7	0
5	B	60	0	0	1	0
5	C	117	0	0	3	0
5	D	62	0	0	0	0
5	E	103	0	0	2	0
5	F	39	0	0	0	0
5	G	100	0	0	1	0
5	H	35	0	0	0	0
All	All	8022	0	7247	93	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 6.

All (93) 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:G:3[A]:LYS:HE2	1:G:5:GLU:HB3	1.24	1.14
1:A:17:GLU:OE2	1:A:30:SER:HB2	1.56	1.04
1:E:80:GLN:HE21	1:E:80:GLN:H	1.14	0.96
1:G:3[A]:LYS:CE	1:G:5:GLU:HB3	2.02	0.89
1:C:43:THR:HG23	2:D:221[B]:LEU:HD22	1.64	0.80
1:E:80:GLN:H	1:E:80:GLN:NE2	1.80	0.79
1:E:80:GLN:HE21	1:E:80:GLN:N	1.80	0.79
1:E:102:ASP:O	1:E:131:LYS:HE2	1.83	0.79
2:B:168:ARG:HH11	2:B:168:ARG:HG3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HZ2	1:C:5:GLU:HG3	1.55	0.71
1:E:52:LYS:HE2	5:E:356:HOH:O	1.92	0.68
1:C:132[B]:GLU:HG3	5:C:156:HOH:O	1.93	0.67
2:H:221[A]:LEU:HD12	2:H:223:PHE:CE2	2.29	0.66
1:A:69:GLN:HG2	2:B:203:TYR:OH	1.97	0.65
1:G:3[B]:LYS:HB2	5:G:283:HOH:O	1.97	0.64
1:E:107:LYS:HB3	4:E:155:PE8:H231	1.80	0.63
1:A:101[A]:LYS:HE2	5:A:629:HOH:O	1.98	0.63
2:B:168:ARG:HD2	2:B:178:LEU:HD12	1.81	0.63
1:E:43:THR:HG23	2:F:221:LEU:HD22	1.82	0.61
5:A:157:HOH:O	1:C:25:HIS:HD2	1.82	0.61
2:B:168:ARG:HH11	2:B:168:ARG:CG	2.14	0.60
1:C:90:GLU:HG3	2:D:189:GLY:HA3	1.83	0.60
1:G:78:MET:HE3	2:H:229:ILE:HD12	1.83	0.60
1:C:126:LYS:HE3	5:C:228:HOH:O	2.02	0.59
1:E:18:LEU:C	1:E:18:LEU:HD23	2.28	0.59
2:B:168:ARG:HD2	2:B:178:LEU:CD1	2.34	0.57
1:E:153:THR:HG22	2:F:162:LYS:HB2	1.90	0.54
1:E:93:VAL:O	2:F:185:ASN:HA	2.07	0.54
1:E:26:LYS:HE2	4:E:155:PE8:H52	1.92	0.52
1:C:3:LYS:NZ	1:C:5:GLU:HG3	2.26	0.51
1:E:14:ILE:HD11	1:E:71:PHE:CE2	2.45	0.51
1:G:69:GLN:HG2	2:H:203:TYR:OH	2.11	0.51
1:E:96:ARG:HA	2:F:182:TYR:O	2.11	0.50
2:B:168:ARG:CG	2:B:168:ARG:NH1	2.75	0.50
2:H:202:SER:O	2:H:224:VAL:HA	2.12	0.50
2:D:170:ASN:HD21	2:H:168[A]:ARG:HH22	1.61	0.49
1:E:26:LYS:HE3	4:E:155:PE8:H81	1.94	0.49
1:A:128:ILE:HD11	5:A:644:HOH:O	2.13	0.49
1:G:31:GLY:HA3	1:G:46:LEU:HD23	1.95	0.49
1:C:3:LYS:HZ3	1:C:5:GLU:H	1.59	0.49
1:C:66:CR2:N2	1:C:66:CR2:HD1	2.28	0.48
1:C:18:LEU:HD23	1:C:19:ASP:N	2.28	0.48
1:C:120:VAL:HG12	1:C:122:ARG:HG3	1.96	0.48
1:E:26:LYS:CE	4:E:155:PE8:H81	2.44	0.48
1:G:53:LEU:HD22	1:G:57:TRP:CD2	2.49	0.48
1:E:38:THR:O	1:E:73:ARG:HD2	2.14	0.47
1:G:18:LEU:HD23	1:G:18:LEU:C	2.39	0.47
1:A:31:GLY:HA3	1:A:46:LEU:HD23	1.97	0.47
1:G:128:ILE:O	1:G:129:ASP:HB2	2.15	0.47
1:A:18:LEU:C	1:A:18:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PHE:CE2	1:C:119:LEU:HD12	2.51	0.46
1:E:53:LEU:HD22	1:E:57:TRP:CE2	2.50	0.46
2:B:161:ILE:HG13	2:B:185:ASN:HB2	1.97	0.46
1:A:126:LYS:HD2	5:A:551:HOH:O	2.15	0.46
1:A:113:LYS:HE2	5:A:162:HOH:O	2.14	0.45
1:E:16:VAL:C	1:E:17:GLU:HG2	2.42	0.45
1:A:25:HIS:HD2	5:A:197:HOH:O	1.99	0.44
1:A:68:LEU:HD21	1:A:121:ASN:HB2	1.98	0.44
1:C:36:ASP:OD2	1:C:38:THR:HB	2.17	0.44
1:C:18:LEU:HD23	1:C:18:LEU:C	2.41	0.44
1:E:112:VAL:HA	1:E:120:VAL:O	2.17	0.44
1:G:80:GLN:H	1:G:80:GLN:CD	2.24	0.44
1:C:151:TYR:O	2:D:163:ALA:HA	2.17	0.44
1:G:68:LEU:HD21	1:G:121:ASN:HB2	1.99	0.44
1:C:18:LEU:HD23	1:C:19:ASP:C	2.43	0.43
1:G:53:LEU:HD22	1:G:57:TRP:CE2	2.53	0.43
1:C:3:LYS:HB2	1:C:4:GLY:H	1.66	0.43
1:E:47:ILE:HD13	2:F:215[A]:ARG:CZ	2.49	0.43
1:A:122[A]:ARG:HG2	1:A:122[A]:ARG:HH11	1.84	0.42
1:C:68:LEU:HD21	1:C:121:ASN:HB2	2.01	0.42
1:E:47:ILE:HG21	2:F:215[A]:ARG:NE	2.34	0.42
1:E:126:LYS:HB2	4:E:155:PE8:H172	2.01	0.42
1:G:68:LEU:HD22	1:G:119:LEU:CD1	2.50	0.42
5:A:157:HOH:O	1:C:25:HIS:CD2	2.65	0.42
1:C:41[A]:LYS:HE2	5:C:160:HOH:O	2.19	0.42
1:C:125:LEU:C	1:C:125:LEU:HD23	2.45	0.42
1:G:29:VAL:HA	1:G:47:ILE:O	2.19	0.42
1:C:70:CYS:SG	1:C:119:LEU:HD11	2.60	0.42
2:D:233:MET:O	2:D:234:ASP:HB2	2.20	0.42
1:E:88:MET:HE1	1:E:112:VAL:HG22	2.02	0.42
1:E:147:SER:HB3	2:F:204:GLN:HG2	2.02	0.42
1:G:125:LEU:C	1:G:125:LEU:HD23	2.45	0.41
1:G:68:LEU:HD22	1:G:119:LEU:HD12	2.02	0.41
1:G:86:SER:HB3	2:H:194:LEU:HD22	2.02	0.41
1:G:112:VAL:HA	1:G:120:VAL:O	2.20	0.41
1:G:41[A]:LYS:NZ	2:H:221[A]:LEU:HD11	2.35	0.41
1:A:26:LYS:O	1:C:50:THR:HA	2.21	0.41
1:E:21:ASP:OD1	1:E:21:ASP:C	2.63	0.41
1:E:52:LYS:CE	5:E:356:HOH:O	2.61	0.41
1:E:66:CR2:N2	1:E:66:CR2:HD1	2.36	0.41
2:B:155:ASP:N	5:B:248:HOH:O	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:PHE:HD2	2:H:206:ALA:HB1	1.86	0.40
1:C:112:VAL:HA	1:C:120:VAL:O	2.22	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	152/173 (88%)	149 (98%)	3 (2%)	0	100	100
1	C	150/173 (87%)	148 (99%)	2 (1%)	0	100	100
1	E	147/173 (85%)	143 (97%)	4 (3%)	0	100	100
1	G	149/173 (86%)	145 (97%)	4 (3%)	0	100	100
2	B	79/93 (85%)	79 (100%)	0	0	100	100
2	D	75/93 (81%)	74 (99%)	1 (1%)	0	100	100
2	F	72/93 (77%)	72 (100%)	0	0	100	100
2	H	72/93 (77%)	71 (99%)	1 (1%)	0	100	100
All	All	896/1064 (84%)	881 (98%)	15 (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	137/150 (91%)	135 (98%)	2 (2%)	57	65
1	C	134/150 (89%)	126 (94%)	8 (6%)	17	15
1	E	131/150 (87%)	123 (94%)	8 (6%)	17	15
1	G	134/150 (89%)	127 (95%)	7 (5%)	21	20
2	B	69/81 (85%)	65 (94%)	4 (6%)	18	16
2	D	65/81 (80%)	63 (97%)	2 (3%)	35	39
2	F	63/81 (78%)	58 (92%)	5 (8%)	11	9
2	H	64/81 (79%)	55 (86%)	9 (14%)	3	2
All	All	797/924 (86%)	752 (94%)	45 (6%)	21	18

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	30	SER
2	B	168	ARG
2	B	176	VAL
2	B	178	LEU
2	B	221	LEU
1	C	3	LYS
1	C	18	LEU
1	C	41[A]	LYS
1	C	41[B]	LYS
1	C	90	GLU
1	C	112	VAL
1	C	119	LEU
1	C	123	ILE
2	D	178	LEU
2	D	214	LYS
1	E	5	GLU
1	E	17	GLU
1	E	42	LEU
1	E	52	LYS
1	E	80	GLN
1	E	112	VAL
1	E	123	ILE
1	E	153	THR
2	F	159	ASN
2	F	176	VAL
2	F	194	LEU

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Mol	Chain	Res	Type
2	F	221	LEU
2	F	230	THR
1	G	3[A]	LYS
1	G	3[B]	LYS
1	G	17	GLU
1	G	73	ARG
1	G	79	LYS
1	G	80	GLN
1	G	112	VAL
2	H	159[A]	ASN
2	H	159[B]	ASN
2	H	168[A]	ARG
2	H	168[B]	ARG
2	H	178	LEU
2	H	180	ASP
2	H	194	LEU
2	H	221[A]	LEU
2	H	221[B]	LEU

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	25	HIS
1	A	135	ASN
1	C	25	HIS
1	C	105	ASN
1	C	135	ASN
2	D	170	ASN
2	D	184	GLN
1	E	80	GLN
2	F	170	ASN
1	G	135	ASN
1	G	149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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$
1	CR2	E	66	1	20,20,21	3.74	6 (30%)	25,27,29	4.00	7 (28%)
1	CR2	C	66	1	20,20,21	3.87	7 (35%)	25,27,29	3.91	8 (32%)
1	CR2	A	66	1	20,20,21	3.77	6 (30%)	25,27,29	2.93	9 (36%)
1	CR2	G	66	1	20,20,21	3.52	6 (30%)	25,27,29	3.27	11 (44%)

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
1	CR2	E	66	1	-	1/6/25/26	0/2/2/2
1	CR2	C	66	1	-	1/6/25/26	0/2/2/2
1	CR2	A	66	1	-	1/6/25/26	0/2/2/2
1	CR2	G	66	1	-	1/6/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CR2	CB2-CA2	13.66	1.48	1.35
1	E	66	CR2	CB2-CA2	13.57	1.48	1.35
1	A	66	CR2	CB2-CA2	12.87	1.47	1.35
1	G	66	CR2	CB2-CA2	11.47	1.46	1.35
1	C	66	CR2	CE1-CZ	7.09	1.52	1.39
1	E	66	CR2	CE1-CZ	7.01	1.52	1.39
1	G	66	CR2	CE1-CZ	6.96	1.52	1.39
1	A	66	CR2	CE1-CZ	6.55	1.51	1.39
1	G	66	CR2	CE1-CD1	4.91	1.46	1.38
1	A	66	CR2	C2-N3	-4.77	1.29	1.40
1	A	66	CR2	CA2-C2	-4.66	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	CR2	C2-N3	-3.89	1.31	1.40
1	A	66	CR2	CE1-CD1	3.89	1.45	1.38
1	C	66	CR2	C1-N2	3.68	1.38	1.32
1	C	66	CR2	CE1-CD1	3.65	1.44	1.38
1	C	66	CR2	O2-C2	3.33	1.29	1.23
1	E	66	CR2	C2-N3	-3.33	1.32	1.40
1	G	66	CR2	CA2-C2	-3.14	1.45	1.48
1	C	66	CR2	CA2-C2	-3.08	1.45	1.48
1	E	66	CR2	CA2-C2	-3.07	1.45	1.48
1	E	66	CR2	CE1-CD1	2.86	1.43	1.38
1	G	66	CR2	O2-C2	2.86	1.28	1.23
1	C	66	CR2	C2-N3	-2.78	1.33	1.40
1	E	66	CR2	C1-N2	2.73	1.37	1.32
1	A	66	CR2	O2-C2	2.03	1.27	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CR2	O2-C2-CA2	-13.50	122.41	131.02
1	E	66	CR2	O2-C2-CA2	-13.40	122.47	131.02
1	G	66	CR2	O2-C2-CA2	-10.04	124.61	131.02
1	C	66	CR2	C2-N3-C1	-7.79	104.58	108.08
1	A	66	CR2	O2-C2-CA2	-7.65	126.14	131.02
1	E	66	CR2	CA2-C2-N3	7.52	109.81	103.50
1	E	66	CR2	C2-N3-C1	-7.46	104.73	108.08
1	C	66	CR2	CA2-C2-N3	7.25	109.59	103.50
1	A	66	CR2	CA2-C2-N3	7.08	109.45	103.50
1	G	66	CR2	CD1-CE1-CZ	-5.73	113.81	119.88
1	E	66	CR2	CD1-CE1-CZ	-5.60	113.96	119.88
1	G	66	CR2	CA2-C2-N3	5.59	108.19	103.50
1	A	66	CR2	C2-N3-C1	-5.45	105.63	108.08
1	E	66	CR2	C1-CA1-N1	-5.41	100.89	112.85
1	A	66	CR2	C1-CA1-N1	-4.91	102.00	112.85
1	G	66	CR2	C2-N3-C1	-4.39	106.10	108.08
1	C	66	CR2	CD1-CE1-CZ	-4.31	115.32	119.88
1	G	66	CR2	C1-CA1-N1	-4.23	103.49	112.85
1	E	66	CR2	CD2-CG2-CD1	4.14	123.79	117.65
1	C	66	CR2	CG2-CB2-CA2	-4.13	124.95	129.87
1	C	66	CR2	C1-CA1-N1	-3.54	105.02	112.85
1	G	66	CR2	CD2-CG2-CD1	3.53	122.89	117.65
1	G	66	CR2	CB2-CA2-C2	3.43	126.51	122.36
1	A	66	CR2	CD1-CE1-CZ	-3.20	116.49	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CR2	CD2-CG2-CD1	3.04	122.16	117.65
1	A	66	CR2	CB2-CA2-C2	2.74	125.68	122.36
1	E	66	CR2	C2-CA2-N2	-2.57	107.11	108.95
1	A	66	CR2	C2-CA2-N2	-2.55	107.13	108.95
1	A	66	CR2	CD2-CG2-CD1	2.54	121.41	117.65
1	A	66	CR2	C3-CA3-N3	2.37	117.83	112.43
1	G	66	CR2	CB2-CA2-N2	-2.26	125.69	128.76
1	C	66	CR2	CA3-N3-C2	2.26	128.64	123.67
1	G	66	CR2	CA1-C1-N3	2.18	125.44	122.52
1	G	66	CR2	CE2-CZ-CE1	2.17	123.22	119.77
1	G	66	CR2	CD2-CG2-CB2	-2.14	113.85	121.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CR2	C3-CA3-N3-C2
1	E	66	CR2	C3-CA3-N3-C2
1	G	66	CR2	C3-CA3-N3-C2
1	A	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	66	CR2	1	0
1	C	66	CR2	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	SO4	C	155	-	4,4,4	0.43	0	6,6,6	0.82	0
4	PE8	E	155	-	24,24,24	1.06	0	23,23,23	0.88	1 (4%)

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	PE8	E	155	-	-	15/22/22/22	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	E	155	PE8	O4-C5-C6	2.23	120.50	110.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

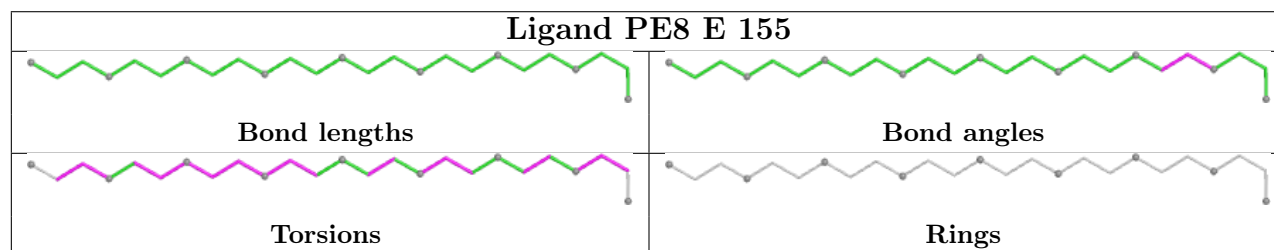
Mol	Chain	Res	Type	Atoms
4	E	155	PE8	O4-C5-C6-O7
4	E	155	PE8	O19-C20-C21-O22
4	E	155	PE8	O10-C11-C12-O13
4	E	155	PE8	O13-C14-C15-O16
4	E	155	PE8	O22-C23-C24-O25
4	E	155	PE8	O1-C2-C3-O4
4	E	155	PE8	O7-C8-C9-O10
4	E	155	PE8	O16-C17-C18-O19
4	E	155	PE8	C2-C3-O4-C5
4	E	155	PE8	C8-C9-O10-C11
4	E	155	PE8	C14-C15-O16-C17
4	E	155	PE8	C17-C18-O19-C20
4	E	155	PE8	C21-C20-O19-C18
4	E	155	PE8	C18-C17-O16-C15
4	E	155	PE8	C24-C23-O22-C21

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	155	PE8	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	152/173 (87%)	-0.73	1 (0%) 84 86	4, 12, 21, 30	5 (3%)
1	C	149/173 (86%)	-0.69	0 100 100	6, 12, 24, 32	5 (3%)
1	E	149/173 (86%)	-0.38	1 (0%) 84 86	6, 18, 32, 44	2 (1%)
1	G	149/173 (86%)	-0.44	2 (1%) 75 77	8, 17, 29, 37	5 (3%)
2	B	80/93 (86%)	-0.60	1 (1%) 75 77	7, 13, 27, 44	1 (1%)
2	D	76/93 (81%)	-0.54	0 100 100	6, 15, 28, 38	1 (1%)
2	F	72/93 (77%)	-0.36	1 (1%) 73 75	7, 18, 36, 41	2 (2%)
2	H	71/93 (76%)	-0.25	2 (2%) 55 57	7, 20, 34, 41	4 (5%)
All	All	898/1064 (84%)	-0.52	8 (0%) 81 83	4, 15, 30, 44	25 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0[A]	MET	4.3
1	E	39	TYR	3.2
1	G	3[A]	LYS	2.8
2	H	229	ILE	2.5
2	H	159[A]	ASN	2.3
2	F	159	ASN	2.2
2	B	234	ASP	2.2
1	G	133	ASP	2.1

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($\text{\AA}^2$)	Q<0.9
1	CR2	A	66	19/20	0.98	0.04	4,7,10,10	0
1	CR2	C	66	19/20	0.98	0.04	2,6,11,12	0
1	CR2	E	66	19/20	0.98	0.04	7,10,14,15	0
1	CR2	G	66	19/20	0.98	0.04	7,12,14,15	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

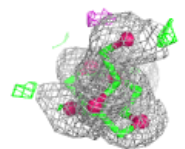
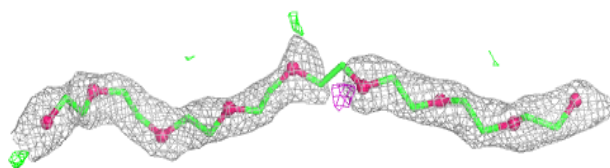
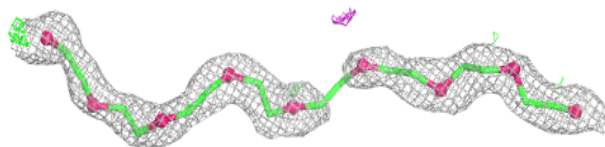
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	PE8	E	155	25/25	0.89	0.14	38,46,49,50	0
3	SO4	C	155	5/5	0.92	0.13	35,35,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PE8 E 155:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.