



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:42 PM UTC

PDB ID : 3NPE / pdb_00003npe
Title : Structure of VP14 in complex with oxygen
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Deposited on : 2010-06-28
Resolution : 3.20 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

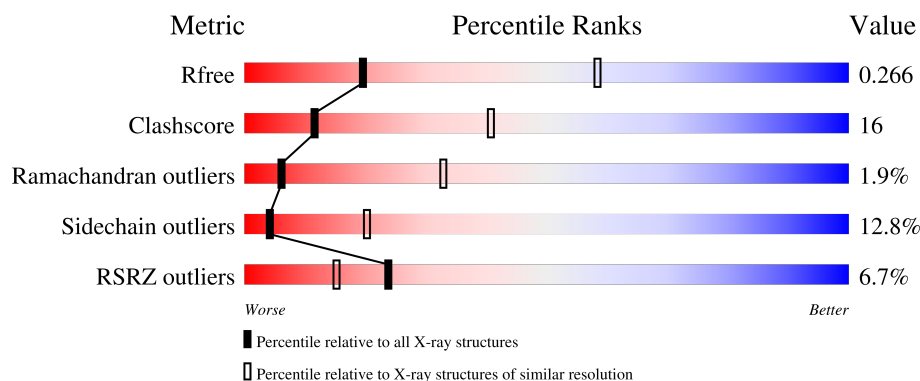
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	529	

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
5	DIO	A	2946	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4042 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.

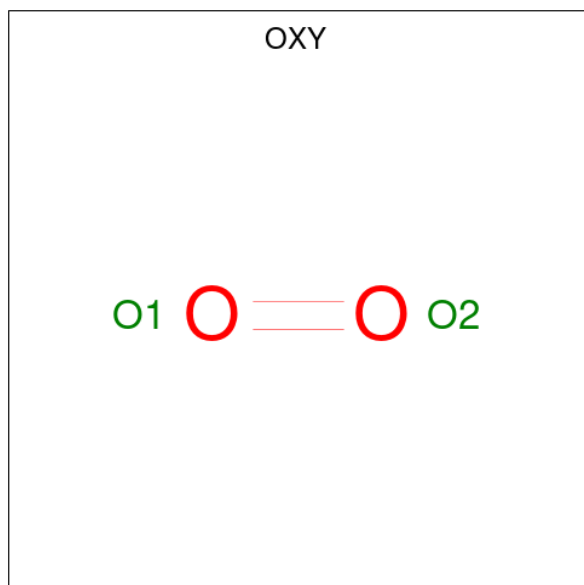
- Molecule 1 is a protein called 9-cis-epoxycarotenoid dioxygenase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4010	2536	704	752	18			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

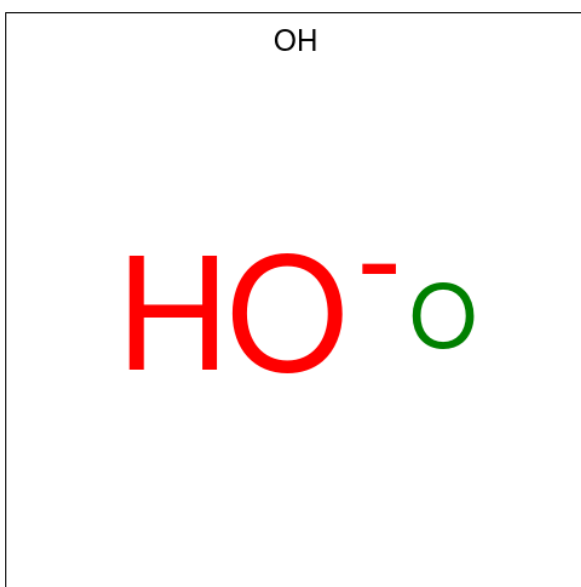
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



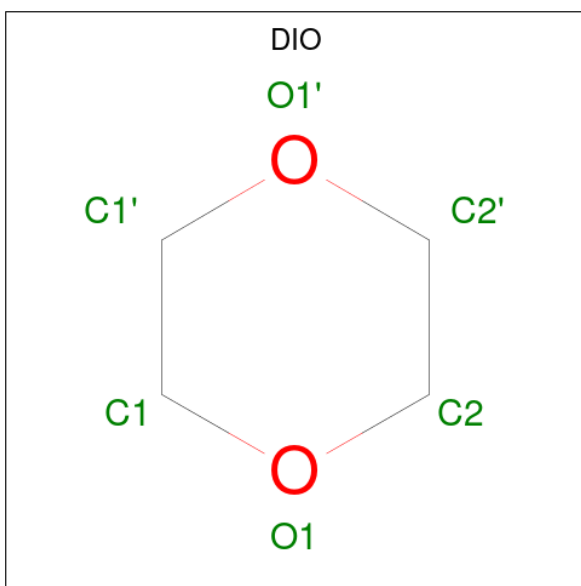
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

- Molecule 4 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		

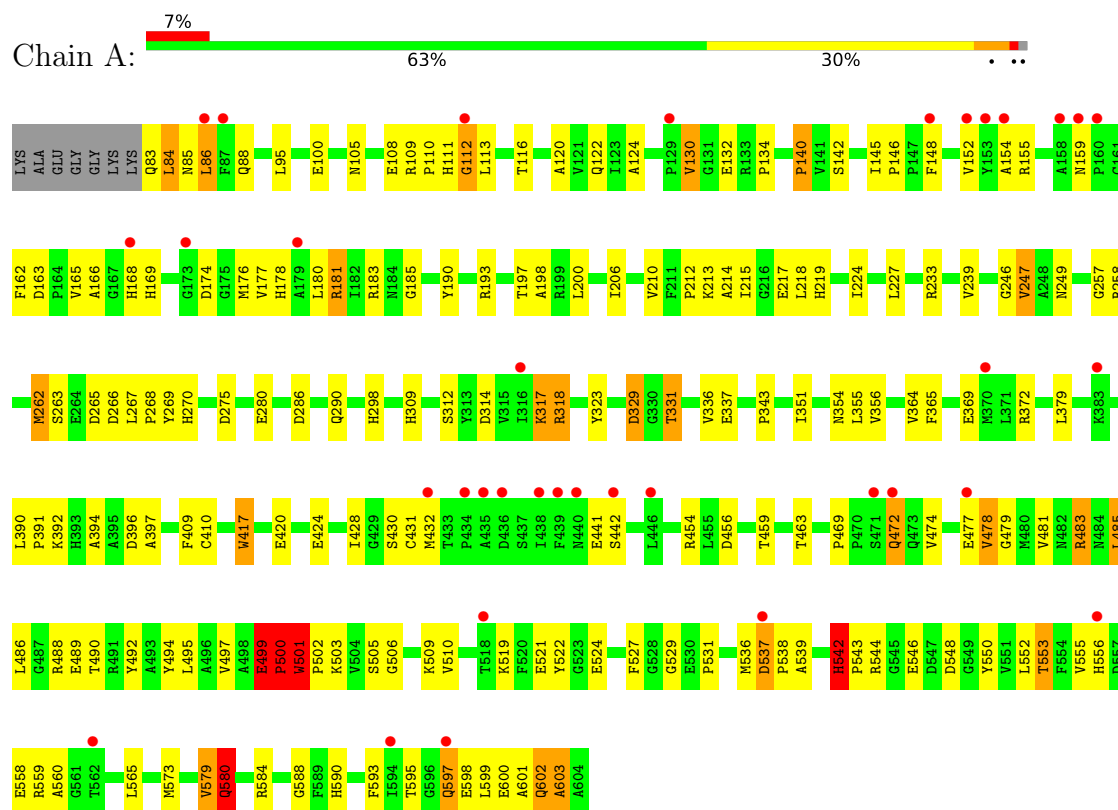
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		

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: 9-cis-epoxycarotenoid dioxygenase 1, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	161.52Å 161.52Å 150.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.30 – 3.20 47.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.30-3.20) 99.6 (47.30-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.272 0.228 , 0.266	Depositor DCC
R_{free} test set	1174 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	101.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 95.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4042	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FE2, OXY, DIO, OH

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	0.73	6/4112 (0.1%)	1.02	14/5598 (0.3%)

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
1	A	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	579	VAL	CB-CG2	7.45	1.77	1.52
1	A	580	GLN	CD-NE2	6.87	1.47	1.33
1	A	140	PRO	C-O	6.84	1.31	1.23
1	A	580	GLN	CD-OE1	6.73	1.36	1.23
1	A	140	PRO	N-CD	6.66	1.57	1.47
1	A	579	VAL	CB-CG1	5.65	1.71	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	GLU	CA-C-N	7.94	129.76	119.84
1	A	499	GLU	C-N-CA	7.94	129.76	119.84
1	A	559	ARG	N-CA-C	-7.67	100.87	111.30
1	A	501	TRP	CA-C-N	-6.39	113.11	119.56
1	A	501	TRP	C-N-CA	-6.39	113.11	119.56
1	A	499	GLU	N-CA-C	5.59	122.18	109.81
1	A	580	GLN	OE1-CD-NE2	5.32	127.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	PRO	N-CA-C	5.29	123.36	112.47
1	A	537	ASP	CB-CA-C	5.16	118.80	109.61
1	A	290	GLN	N-CA-C	5.16	116.71	111.14
1	A	527	PHE	N-CA-C	5.13	117.18	109.23
1	A	86	LEU	N-CA-C	-5.12	106.98	113.43
1	A	105	ASN	N-CA-C	5.11	117.75	111.82
1	A	140	PRO	N-CD-CG	-5.03	95.66	103.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	GLU	Peptide
1	A	500	PRO	Peptide
1	A	537	ASP	Peptide
1	A	542	HIS	Peptide
1	A	558	GLU	Peptide
1	A	560	ALA	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	4010	0	3875	127	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	18	0	24	6	0
6	A	10	0	0	0	0
All	All	4042	0	3899	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (127) 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:579:VAL:CB	1:A:579:VAL:CG2	1.77	1.59
1:A:148:PHE:HZ	1:A:550:TYR:CE2	1.70	1.09
1:A:148:PHE:CZ	1:A:550:TYR:HE2	1.78	1.01
1:A:130:VAL:HG23	1:A:584:ARG:HH21	1.25	0.98
1:A:509:LYS:HB2	1:A:573:MET:HE3	1.42	0.98
1:A:148:PHE:HZ	1:A:550:TYR:HE2	0.93	0.92
1:A:262:MET:HA	1:A:262:MET:HE2	1.52	0.92
1:A:148:PHE:CZ	1:A:550:TYR:CE2	2.53	0.90
1:A:474:VAL:HG13	1:A:499:GLU:HG3	1.60	0.83
1:A:193:ARG:HH22	5:A:2946:DIO:H2'2	1.41	0.83
1:A:479:GLY:HA3	1:A:495:LEU:HD23	1.61	0.82
1:A:162:PHE:HA	5:A:2948:DIO:H2'2	1.62	0.81
1:A:130:VAL:HG12	1:A:176:MET:HE1	1.62	0.80
1:A:391:PRO:HG2	1:A:394:ALA:HB2	1.63	0.80
1:A:390:LEU:HD12	1:A:391:PRO:HD2	1.65	0.79
1:A:485:LEU:CD2	1:A:546:GLU:HG3	2.19	0.73
1:A:168:HIS:HD2	1:A:213:LYS:HD2	1.59	0.68
1:A:116:THR:HG21	1:A:441:GLU:HB3	1.76	0.67
1:A:262:MET:HA	1:A:262:MET:CE	2.22	0.67
1:A:509:LYS:CB	1:A:573:MET:HE3	2.22	0.67
1:A:536:MET:HG2	1:A:548:ASP:O	1.94	0.66
1:A:354:ASN:C	1:A:355:LEU:HD12	2.20	0.66
1:A:329:ASP:N	1:A:329:ASP:OD1	2.29	0.66
1:A:579:VAL:CG2	1:A:579:VAL:CA	2.71	0.66
1:A:509:LYS:HD2	1:A:573:MET:HE3	1.78	0.65
1:A:337:GLU:O	1:A:397:ALA:HB2	1.97	0.64
1:A:163:ASP:HB2	5:A:2948:DIO:H1'1	1.82	0.61
1:A:595:THR:HB	1:A:598:GLU:HB2	1.81	0.61
1:A:134:PRO:HG2	5:A:2946:DIO:H1'1	1.82	0.61
1:A:474:VAL:HG13	1:A:499:GLU:CG	2.31	0.60
1:A:116:THR:HA	1:A:122:GLN:NE2	2.16	0.60
1:A:134:PRO:CG	5:A:2946:DIO:H1'1	2.31	0.60
1:A:509:LYS:HD2	1:A:573:MET:CE	2.31	0.59
1:A:483:ARG:HH12	1:A:593:PHE:HB3	1.68	0.59
1:A:483:ARG:HH22	1:A:593:PHE:H	1.52	0.58
1:A:109:ARG:N	1:A:110:PRO:HD2	2.19	0.57
1:A:266:ASP:OD1	1:A:267:LEU:N	2.38	0.57
1:A:354:ASN:HB2	1:A:355:LEU:HD12	1.87	0.57
1:A:146:PRO:HB3	1:A:148:PHE:CE2	2.40	0.57
1:A:262:MET:HE1	1:A:268:PRO:HG3	1.87	0.56
1:A:329:ASP:HB2	1:A:331:THR:OG1	2.06	0.55
1:A:215:ILE:O	1:A:219:HIS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA3	1:A:266:ASP:HB2	1.87	0.55
1:A:130:VAL:HG23	1:A:584:ARG:NH2	2.07	0.54
1:A:176:MET:HG3	1:A:193:ARG:O	2.07	0.54
1:A:120:ALA:O	1:A:124:ALA:HB2	2.07	0.54
1:A:134:PRO:CB	5:A:2946:DIO:H1'1	2.37	0.54
1:A:146:PRO:HG2	1:A:550:TYR:CZ	2.43	0.54
1:A:424:GLU:OE1	1:A:454:ARG:NH1	2.40	0.53
1:A:180:LEU:HD23	1:A:565:LEU:HD22	1.88	0.53
1:A:111:HIS:O	1:A:112:GLY:O	2.27	0.53
1:A:85:ASN:CG	1:A:86:LEU:H	2.16	0.53
1:A:355:LEU:HG	1:A:391:PRO:HA	1.90	0.53
1:A:494:TYR:CE1	1:A:509:LYS:HG3	2.43	0.53
1:A:555:VAL:HG12	1:A:556:HIS:N	2.25	0.52
1:A:140:PRO:HG2	1:A:580:GLN:HB2	1.92	0.52
1:A:390:LEU:CD1	1:A:391:PRO:HD2	2.39	0.52
1:A:552:LEU:HB3	1:A:565:LEU:HD11	1.93	0.51
1:A:109:ARG:N	1:A:110:PRO:CD	2.74	0.51
1:A:146:PRO:CB	1:A:148:PHE:CE2	2.94	0.51
1:A:116:THR:HG21	1:A:441:GLU:CB	2.41	0.50
1:A:174:ASP:HA	1:A:247:VAL:HG22	1.92	0.50
1:A:85:ASN:HB3	1:A:88:GLN:HG2	1.94	0.50
1:A:509:LYS:HB2	1:A:573:MET:CE	2.29	0.50
1:A:176:MET:HG3	1:A:193:ARG:C	2.36	0.50
1:A:469:PRO:HG2	1:A:472:GLN:NE2	2.27	0.50
1:A:108:GLU:C	1:A:110:PRO:HD2	2.37	0.49
1:A:474:VAL:HG11	1:A:497:VAL:HG13	1.93	0.49
1:A:369:GLU:OE2	1:A:372:ARG:NH2	2.45	0.49
1:A:178:HIS:CD2	1:A:190:TYR:OH	2.64	0.49
1:A:178:HIS:HD2	1:A:190:TYR:OH	1.96	0.49
1:A:485:LEU:HD23	1:A:546:GLU:HG3	1.92	0.49
1:A:246:GLY:HA3	1:A:266:ASP:CB	2.43	0.49
1:A:180:LEU:HD23	1:A:565:LEU:CD2	2.44	0.48
1:A:553:THR:C	1:A:565:LEU:HD12	2.39	0.48
1:A:317:LYS:NZ	1:A:318:ARG:HG2	2.28	0.48
1:A:218:LEU:CD2	1:A:227:LEU:HD13	2.44	0.48
1:A:309:HIS:CD2	1:A:351:ILE:HD11	2.49	0.47
1:A:257:GLY:O	1:A:602:GLN:HA	2.14	0.47
1:A:176:MET:HE3	1:A:178:HIS:CE1	2.49	0.47
1:A:542:HIS:HB2	1:A:543:PRO:CD	2.45	0.47
1:A:485:LEU:HD21	1:A:546:GLU:HG3	1.95	0.47
1:A:492:TYR:HA	1:A:510:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:HIS:CE1	1:A:392:LYS:HD2	2.50	0.46
1:A:298:HIS:HE1	1:A:590:HIS:CE1	2.34	0.46
1:A:152:VAL:HG23	1:A:599:LEU:HD11	1.96	0.46
1:A:424:GLU:HG2	1:A:456:ASP:HB2	1.98	0.46
1:A:501:TRP:HB3	1:A:502:PRO:HD3	1.97	0.46
1:A:500:PRO:O	1:A:501:TRP:C	2.58	0.46
1:A:258:ARG:HG2	1:A:270:HIS:CE1	2.51	0.46
1:A:601:ALA:O	1:A:602:GLN:C	2.59	0.46
1:A:145:ILE:HB	1:A:185:GLY:HA2	1.98	0.45
1:A:485:LEU:HB3	1:A:490:THR:CG2	2.46	0.45
1:A:343:PRO:HB2	1:A:365:PHE:HB2	1.99	0.45
1:A:122:GLN:HG3	1:A:169:HIS:HA	1.98	0.45
1:A:154:ALA:HA	1:A:178:HIS:O	2.16	0.45
1:A:212:PRO:HA	1:A:217:GLU:OE1	2.16	0.45
1:A:181:ARG:HH12	1:A:183:ARG:CZ	2.30	0.45
1:A:249:ASN:OD1	1:A:249:ASN:C	2.60	0.44
1:A:181:ARG:HH12	1:A:183:ARG:NH1	2.14	0.44
1:A:146:PRO:HG2	1:A:550:TYR:CE1	2.52	0.44
1:A:265:ASP:OD1	1:A:265:ASP:N	2.51	0.44
1:A:85:ASN:CB	1:A:88:GLN:HG2	2.48	0.44
1:A:477:GLU:OE2	1:A:501:TRP:CH2	2.70	0.44
1:A:417:TRP:CG	1:A:489:GLU:HA	2.53	0.43
1:A:146:PRO:HB3	1:A:148:PHE:HE2	1.78	0.43
1:A:214:ALA:O	1:A:218:LEU:HB2	2.18	0.43
1:A:556:HIS:CE1	1:A:584:ARG:HG3	2.53	0.43
1:A:323:TYR:CE1	1:A:356:VAL:HG21	2.54	0.43
1:A:155:ARG:CZ	1:A:588:GLY:HA3	2.49	0.43
1:A:409:PHE:O	1:A:431:CYS:HB3	2.18	0.43
1:A:536:MET:O	1:A:536:MET:HG3	2.18	0.43
1:A:477:GLU:HB3	1:A:478:VAL:H	1.65	0.42
1:A:602:GLN:O	1:A:603:ALA:O	2.38	0.42
1:A:197:THR:O	1:A:200:LEU:N	2.53	0.42
1:A:165:VAL:O	1:A:166:ALA:C	2.63	0.41
1:A:597:GLN:HA	1:A:600:GLU:HG3	2.02	0.41
1:A:130:VAL:H	1:A:159:ASN:HD21	1.67	0.41
1:A:197:THR:HA	1:A:269:TYR:CE2	2.56	0.41
1:A:95:LEU:HD13	1:A:233:ARG:CG	2.51	0.41
1:A:529:GLY:O	1:A:531:PRO:HD3	2.21	0.41
1:A:542:HIS:CB	1:A:543:PRO:HD3	2.50	0.41
1:A:542:HIS:CB	1:A:543:PRO:CD	2.99	0.41
1:A:506:GLY:HA2	1:A:522:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:HIS:HB2	1:A:543:PRO:HD3	2.03	0.41
1:A:474:VAL:CG1	1:A:497:VAL:HG13	2.52	0.40
1:A:555:VAL:CG1	1:A:556:HIS:N	2.84	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	520/529 (98%)	461 (89%)	49 (9%)	10 (2%)	6	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	PRO
1	A	501	TRP
1	A	539	ALA
1	A	603	ALA
1	A	112	GLY
1	A	542	HIS
1	A	84	LEU
1	A	198	ALA
1	A	442	SER
1	A	478	VAL

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	415/419 (99%)	362 (87%)	53 (13%)	4 20

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	84	LEU
1	A	100	GLU
1	A	113	LEU
1	A	130	VAL
1	A	132	GLU
1	A	142	SER
1	A	177	VAL
1	A	181	ARG
1	A	206	ILE
1	A	210	VAL
1	A	224	ILE
1	A	239	VAL
1	A	247	VAL
1	A	262	MET
1	A	263	SER
1	A	275	ASP
1	A	280	GLU
1	A	286	ASP
1	A	312	SER
1	A	314	ASP
1	A	317	LYS
1	A	318	ARG
1	A	329	ASP
1	A	331	THR
1	A	336	VAL
1	A	364	VAL
1	A	379	LEU
1	A	396	ASP
1	A	410	CYS
1	A	417	TRP
1	A	420	GLU
1	A	428	ILE
1	A	430	SER
1	A	432	MET
1	A	459	THR

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Mol	Chain	Res	Type
1	A	463	THR
1	A	472	GLN
1	A	481	VAL
1	A	483	ARG
1	A	485	LEU
1	A	486	LEU
1	A	488	ARG
1	A	503	LYS
1	A	505	SER
1	A	519	LYS
1	A	521	GLU
1	A	524	GLU
1	A	544	ARG
1	A	553	THR
1	A	580	GLN
1	A	597	GLN
1	A	602	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	137	HIS
1	A	168	HIS
1	A	169	HIS
1	A	178	HIS
1	A	219	HIS
1	A	270	HIS
1	A	309	HIS
1	A	472	GLN
1	A	473	GLN
1	A	484	ASN
1	A	556	HIS
1	A	569	ASN

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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic and 1 is modelled with single atom - leaving 4 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	$\# Z > 2$
5	DIO	A	2948	-	6,6,6	1.21	0	6,6,6	0.76	0
3	OXY	A	1	2	1,1,1	0.13	0	-		
5	DIO	A	2947	-	6,6,6	0.79	0	6,6,6	0.95	0
5	DIO	A	2946	-	6,6,6	1.17	0	6,6,6	1.03	1 (16%)

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
5	DIO	A	2948	-	-	-	0/1/1/1
5	DIO	A	2946	-	-	-	0/1/1/1
5	DIO	A	2947	-	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2946	DIO	C2'-O1'-C1'	2.32	117.37	109.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2948	DIO	2	0
5	A	2946	DIO	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/529 (98%)	0.42	35 (6%) 24 15	70, 96, 145, 255	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	6.1
1	A	438	ILE	5.0
1	A	129	PRO	5.0
1	A	439	PHE	4.5
1	A	159	ASN	4.4
1	A	86	LEU	3.9
1	A	148	PHE	3.7
1	A	477	GLU	3.6
1	A	472	GLN	3.5
1	A	435	ALA	3.5
1	A	432	MET	3.4
1	A	173	GLY	3.4
1	A	160	PRO	3.3
1	A	434	PRO	3.2
1	A	537	ASP	3.2
1	A	436	ASP	3.1
1	A	440	ASN	3.1
1	A	158	ALA	3.0
1	A	179	ALA	2.7
1	A	594	ILE	2.6
1	A	87	PHE	2.6
1	A	442	SER	2.6
1	A	562	THR	2.4
1	A	154	ALA	2.4
1	A	370	MET	2.3
1	A	518	THR	2.2
1	A	556	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	597	GLN	2.2
1	A	383	LYS	2.2
1	A	316	ILE	2.1
1	A	471	SER	2.1
1	A	152	VAL	2.1
1	A	446	LEU	2.1
1	A	168	HIS	2.1
1	A	153	TYR	2.1

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($\text{\AA}^2$)	Q<0.9
5	DIO	A	2946	6/6	0.72	0.25	152,153,157,157	0
5	DIO	A	2948	6/6	0.77	0.22	142,143,144,145	0
5	DIO	A	2947	6/6	0.87	0.25	125,126,127,128	0
3	OXY	A	1	2/2	0.97	0.09	72,72,72,73	0
4	OH	A	2	1/1	0.98	0.08	72,72,72,72	0
2	FE2	A	605	1/1	1.00	0.01	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.