



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 4OPE / pdb_00004ope
Title : Streptomyces albus JA3453 oxazolomycin ketosynthase domain OzmH KS7
Authors : Osipiuk, J.; Mack, J.; Endres, M.; Babnigg, G.; Bingman, C.A.; Yennamalli, R.; Lohman, J.R.; Ma, M.; Shen, B.; Phillips Jr., G.N.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2014-02-05
Resolution : 2.58 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

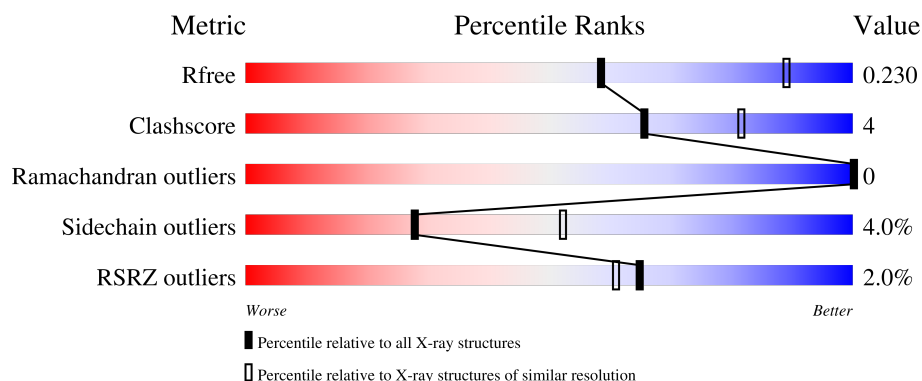
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	587	
1	B	587	
1	C	587	
1	D	587	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17479 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 NRPS/PKS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	Se	0	2	0
			4351	2721	800	817	7	6			
1	B	568	Total	C	N	O	S	Se	0	1	0
			4257	2667	778	799	7	6			
1	C	576	Total	C	N	O	S	Se	0	1	0
			4329	2709	796	811	7	6			
1	D	560	Total	C	N	O	S	Se	0	0	0
			4205	2635	770	787	7	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4218	SER	-	expression tag	UNP B2WW42
A	4219	ASN	-	expression tag	UNP B2WW42
A	4220	ALA	-	expression tag	UNP B2WW42
B	4218	SER	-	expression tag	UNP B2WW42
B	4219	ASN	-	expression tag	UNP B2WW42
B	4220	ALA	-	expression tag	UNP B2WW42
C	4218	SER	-	expression tag	UNP B2WW42
C	4219	ASN	-	expression tag	UNP B2WW42
C	4220	ALA	-	expression tag	UNP B2WW42
D	4218	SER	-	expression tag	UNP B2WW42
D	4219	ASN	-	expression tag	UNP B2WW42
D	4220	ALA	-	expression tag	UNP B2WW42

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



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

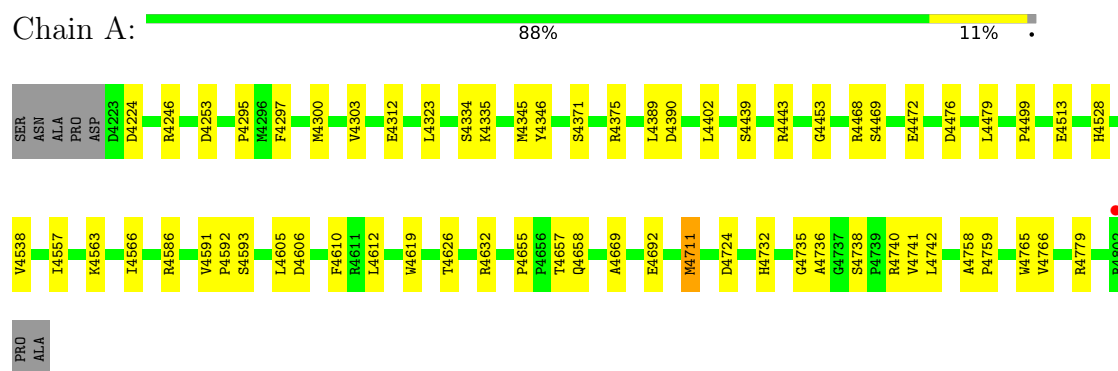
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total	O	0	0
			176	176		
3	B	47	Total	O	0	0
			47	47		
3	C	69	Total	O	0	0
			69	69		
3	D	37	Total	O	0	0
			37	37		

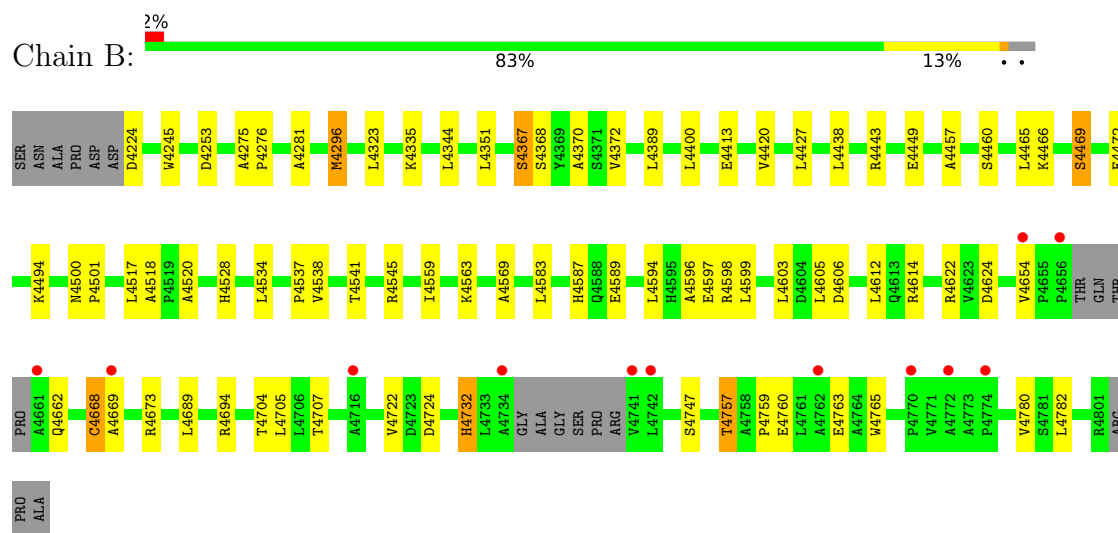
3 Residue-property plots

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.

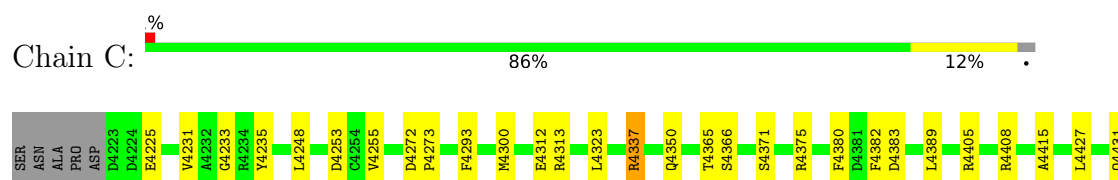
• Molecule 1: NRPS/PKS

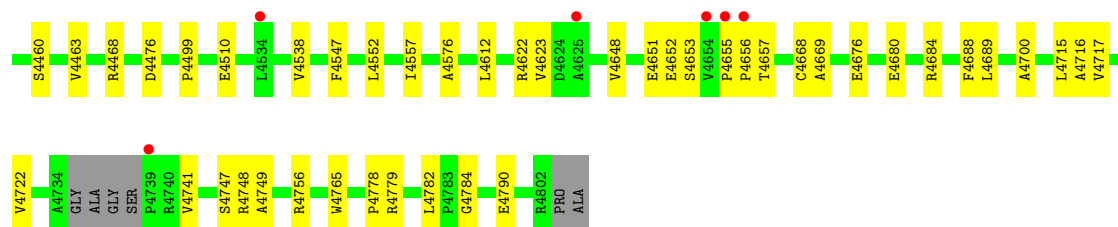


• Molecule 1: NRPS/PKS

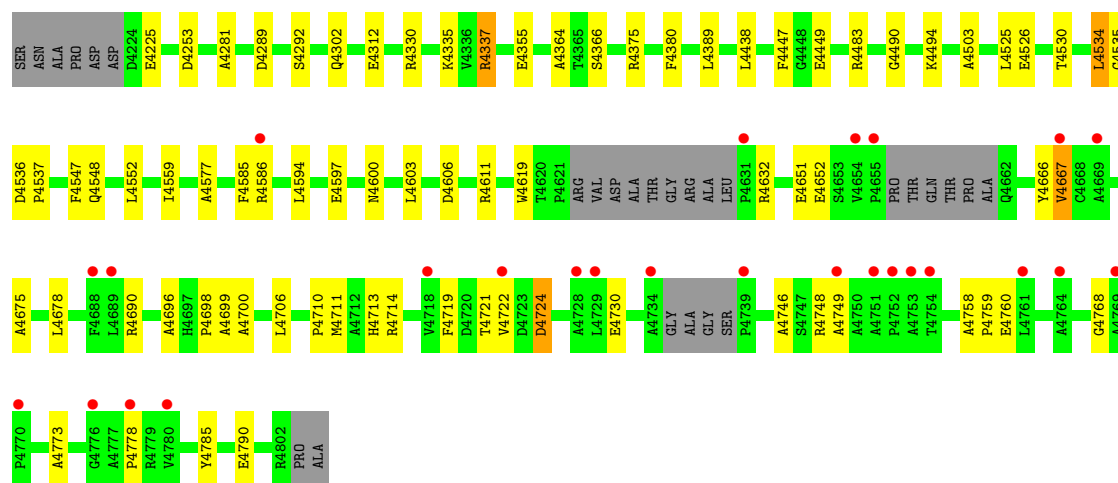
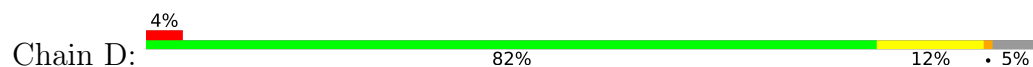


• Molecule 1: NRPS/PKS





Molecule 1: NRPS/PKS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.31Å 139.83Å 173.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.08 – 2.58 41.08 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.08-2.58) 99.5 (41.08-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.177 , 0.231 0.180 , 0.230	Depositor DCC
R_{free} test set	5180 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17479	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: NO3

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	1.05	2/4454 (0.0%)	0.99	3/6053 (0.0%)
1	B	0.83	0/4354	0.94	3/5916 (0.1%)
1	C	0.85	0/4429	0.96	3/6019 (0.0%)
1	D	0.81	0/4298	0.93	2/5835 (0.0%)
All	All	0.89	2/17535 (0.0%)	0.96	11/23823 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4655	PRO	CA-C	6.26	1.55	1.51
1	A	4334	SER	C-O	-5.31	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4597	GLU	N-CA-C	-5.97	104.77	111.28
1	B	4597	GLU	N-CA-C	-5.61	104.86	110.97
1	C	4557	ILE	N-CA-C	5.53	113.51	107.60
1	C	4415	ALA	N-CA-C	5.51	117.64	108.99
1	A	4711	MSE	N-CA-CB	-5.25	101.83	110.65
1	C	4431	GLN	CB-CA-C	-5.13	102.82	110.88
1	B	4296	MSE	N-CA-C	-5.12	105.39	110.97
1	A	4566	ILE	CB-CA-C	-5.10	105.32	110.88
1	D	4675	ALA	N-CA-C	5.09	116.82	111.28
1	B	4351	LEU	N-CA-C	-5.08	106.59	112.89
1	A	4297	PHE	N-CA-C	-5.06	105.67	111.14

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	4351	0	4247	26	0
1	B	4257	0	4150	33	0
1	C	4329	0	4226	37	0
1	D	4205	0	4097	36	0
2	C	8	0	0	0	0
3	A	176	0	0	3	0
3	B	47	0	0	0	0
3	C	69	0	0	0	0
3	D	37	0	0	0	0
All	All	17479	0	16720	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 4.

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:B:4224:ASP:OD2	1:B:4469:SER:OG	2.11	0.68
1:C:4689:LEU:HD22	1:C:4722:VAL:HG13	1.79	0.64
1:C:4669:ALA:HB1	1:C:4765:TRP:CE2	2.33	0.64
1:C:4312:GLU:OE2	1:C:4375:ARG:NH1	2.31	0.63
1:A:4658:GLN:OE1	1:A:4658:GLN:N	2.30	0.59
1:D:4700:ALA:HB2	1:D:4778:PRO:HG2	1.83	0.59
1:B:4669:ALA:HB1	1:B:4765:TRP:CE2	2.38	0.59
1:C:4225:GLU:OE2	1:C:4468:ARG:NH1	2.36	0.58
1:A:4468:ARG:HD3	1:A:4472:GLU:OE2	2.04	0.58
1:D:4534:LEU:HD23	1:D:4535:GLY:N	2.20	0.57
1:B:4253:ASP:OD2	1:B:4443:ARG:NH2	2.38	0.57
1:D:4696:ALA:O	1:D:4722:VAL:HG21	2.03	0.57
1:B:4704:THR:O	1:B:4707:THR:OG1	2.21	0.56
1:C:4684:ARG:NH1	1:C:4784:GLY:O	2.38	0.56
1:D:4547:PHE:HB3	1:D:4552:LEU:HD11	1.86	0.56
1:D:4746:ALA:HB1	1:D:4768:GLY:HA3	1.86	0.56
1:C:4337:ARG:HG2	1:C:4383:ASP:OD1	2.05	0.56
1:C:4476:ASP:HA	1:C:4779:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4668:CYS:O	1:C:4716:ALA:HA	2.06	0.55
1:A:4389:LEU:HD22	1:A:4402:LEU:HD12	1.89	0.54
1:C:4717:VAL:CG2	1:C:4741:VAL:HG22	2.37	0.54
1:C:4380:PHE:HB3	1:C:4382:PHE:CZ	2.42	0.54
1:B:4757:THR:HG23	1:B:4760:GLU:OE1	2.08	0.53
1:A:4742:LEU:HB2	1:A:4766:VAL:HG21	1.91	0.53
1:C:4300:MSE:HE1	1:C:4375:ARG:HD3	1.90	0.53
1:D:4606:ASP:HA	1:D:4611:ARG:NH2	2.23	0.53
1:B:4520:ALA:O	1:B:4622:ARG:NH1	2.41	0.53
1:D:4525:LEU:HD12	1:D:4559:ILE:HG13	1.89	0.53
1:A:4499:PRO:HB2	1:A:4538:VAL:HG11	1.91	0.52
1:B:4494:LYS:NZ	1:C:4255:VAL:O	2.37	0.52
1:C:4688:PHE:CE2	1:C:4782:LEU:HD23	2.45	0.52
1:B:4705:LEU:HG	1:B:4782:LEU:HD12	1.92	0.51
1:B:4596:ALA:O	1:B:4614:ARG:NH1	2.44	0.51
1:B:4281:ALA:HB3	1:B:4438:LEU:HD13	1.93	0.51
1:C:4427:LEU:HD11	1:D:4364:ALA:HB1	1.93	0.50
1:D:4312:GLU:OE2	1:D:4375:ARG:NE	2.36	0.50
1:B:4528:HIS:O	1:B:4563:LYS:HE2	2.11	0.50
1:B:4759:PRO:O	1:B:4763:GLU:HG3	2.11	0.50
1:D:4678:LEU:HD22	1:D:4713:HIS:HB3	1.93	0.50
1:B:4344:LEU:HD21	1:B:4372:VAL:HG21	1.94	0.50
1:D:4711:MSE:SE	1:D:4785:TYR:CE2	3.15	0.49
1:A:4345:MSE:HE2	1:A:4346:TYR:CZ	2.48	0.49
1:D:4706:LEU:HB3	1:D:4773:ALA:HB2	1.95	0.49
1:C:4717:VAL:HG22	1:C:4741:VAL:HG22	1.95	0.49
1:C:4747:SER:OG	1:C:4748:ARG:O	2.28	0.49
1:D:4606:ASP:HA	1:D:4611:ARG:HH22	1.77	0.49
1:C:4235:TYR:CE1	1:C:4576:ALA:HB2	2.49	0.48
1:A:4295:PRO:HD2	3:A:4916:HOH:O	2.12	0.48
1:B:4732:HIS:ND1	1:B:4732:HIS:C	2.70	0.48
1:A:4439:SER:HB3	1:A:4453:GLY:C	2.39	0.48
1:A:4724:ASP:OD1	1:A:4740:ARG:NH2	2.47	0.47
1:A:4476:ASP:HA	1:A:4779:ARG:NH2	2.29	0.47
1:C:4405:ARG:HD2	1:C:4408:ARG:NH1	2.29	0.47
1:C:4651:GLU:HG2	1:C:4652:GLU:N	2.30	0.47
1:A:4224:ASP:OD2	1:A:4469:SER:OG	2.24	0.47
1:B:4517:LEU:HG	1:B:4518:ALA:N	2.29	0.47
1:D:4619:TRP:CD2	1:D:4632:ARG:HD3	2.50	0.47
1:D:4330:ARG:HD3	1:D:4380:PHE:HA	1.97	0.47
1:D:4600:ASN:HB3	1:D:4603:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4619:TRP:CD2	1:A:4632:ARG:HD3	2.50	0.46
1:B:4599:LEU:HD13	1:B:4605:LEU:HD12	1.96	0.46
1:B:4400:LEU:HD12	1:B:4465:LEU:HD11	1.96	0.46
1:C:4231:VAL:HG23	1:C:4463:VAL:HG12	1.98	0.46
1:C:4233:GLY:HA2	1:C:4460:SER:O	2.15	0.46
1:B:4494:LYS:HE2	1:C:4253:ASP:CG	2.40	0.46
1:B:4420:VAL:HG23	1:B:4460:SER:HB2	1.96	0.46
1:C:4293:PHE:CD1	1:C:4313:ARG:HB3	2.50	0.46
1:C:4350:GLN:HA	1:C:4365:THR:OG1	2.16	0.46
1:C:4669:ALA:HB1	1:C:4765:TRP:CD2	2.51	0.46
1:D:4253:ASP:OD1	1:D:4253:ASP:C	2.59	0.46
1:A:4253:ASP:OD2	1:A:4443:ARG:NH2	2.49	0.46
1:B:4668:CYS:O	1:B:4668:CYS:SG	2.74	0.45
1:D:4536:ASP:HB2	1:D:4537:PRO:HD3	1.98	0.45
1:A:4586:ARG:NH1	3:A:5055:HOH:O	2.32	0.45
1:B:4245:TRP:CE3	1:B:4583:LEU:HB3	2.51	0.45
1:B:4541:THR:O	1:B:4545:ARG:HG3	2.17	0.45
1:C:4499:PRO:HB2	1:C:4538:VAL:HG11	1.99	0.45
1:D:4585:PHE:O	1:D:4586:ARG:C	2.60	0.45
1:D:4710:PRO:HB2	1:D:4714:ARG:NH1	2.31	0.45
1:B:4689:LEU:HD22	1:B:4722:VAL:HG13	1.99	0.45
1:D:4748:ARG:O	1:D:4749:ALA:HB3	2.17	0.45
1:B:4612:LEU:HD22	1:B:4614:ARG:HG2	1.99	0.44
1:D:4289:ASP:OD2	1:D:4292:SER:OG	2.25	0.44
1:A:4711:MSE:HE3	3:A:4920:HOH:O	2.18	0.44
1:C:4680:GLU:O	1:C:4684:ARG:HG3	2.18	0.43
1:C:4656:PRO:O	1:C:4657:THR:C	2.60	0.43
1:B:4457:ALA:O	1:B:4569:ALA:HA	2.18	0.43
1:C:4717:VAL:HG21	1:C:4741:VAL:HG22	1.99	0.43
1:C:4748:ARG:O	1:C:4749:ALA:HB3	2.18	0.43
1:D:4281:ALA:HB3	1:D:4438:LEU:HD13	2.01	0.43
1:A:4732:HIS:CD2	1:A:4741:VAL:HG11	2.54	0.43
1:A:4735:GLY:O	1:A:4736:ALA:C	2.62	0.43
1:B:4367:SER:O	1:B:4368:SER:C	2.61	0.43
1:D:4666:TYR:CE2	1:D:4698:PRO:HB2	2.54	0.43
1:A:4312:GLU:OE2	1:A:4375:ARG:HD2	2.19	0.43
1:D:4721:THR:N	1:D:4724:ASP:OD2	2.49	0.43
1:A:4669:ALA:HB1	1:A:4765:TRP:CE2	2.54	0.42
1:B:4534:LEU:O	1:B:4538:VAL:HG23	2.19	0.42
1:D:4483:ARG:NH1	1:D:4651:GLU:OE1	2.52	0.42
1:C:4715:LEU:HD23	1:C:4715:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4490:GLY:HA2	1:D:4503:ALA:CB	2.49	0.42
1:A:4390:ASP:CG	1:B:4370:ALA:HB2	2.45	0.42
1:C:4272:ASP:HA	1:C:4273:PRO:HD3	1.89	0.42
1:D:4690:ARG:NE	1:D:4730:GLU:OE1	2.49	0.42
1:A:4591:VAL:HB	1:A:4592:PRO:HD2	2.01	0.42
1:A:4758:ALA:N	1:A:4759:PRO:CD	2.83	0.42
1:D:4526:GLU:HG2	1:D:4577:ALA:HB1	2.01	0.41
1:C:4653:SER:O	1:C:4655:PRO:HD3	2.20	0.41
1:D:4667:VAL:C	1:D:4719:PHE:HE1	2.28	0.41
1:A:4738:SER:HB3	1:A:4741:VAL:HG23	2.03	0.41
1:A:4557:ILE:O	1:A:4610:PHE:HA	2.21	0.41
1:C:4700:ALA:HA	1:C:4778:PRO:O	2.20	0.41
1:D:4447:PHE:HB3	1:D:4603:LEU:HD11	2.02	0.41
1:D:4632:ARG:NH1	1:D:4652:GLU:OE1	2.53	0.41
1:A:4528:HIS:O	1:A:4563:LYS:HD2	2.20	0.41
1:D:4490:GLY:HA2	1:D:4503:ALA:HB2	2.03	0.41
1:A:4605:LEU:HD22	1:A:4610:PHE:HB2	2.02	0.41
1:B:4500:ASN:HA	1:B:4501:PRO:HD2	1.89	0.41
1:B:4559:ILE:O	1:B:4612:LEU:HA	2.21	0.41
1:B:4587:HIS:O	1:B:4589:GLU:HG3	2.21	0.41
1:B:4534:LEU:C	1:B:4537:PRO:HD2	2.45	0.41
1:D:4758:ALA:N	1:D:4759:PRO:HD2	2.36	0.41
1:C:4510:GLU:CD	1:D:4337:ARG:HH12	2.28	0.40
1:B:4275:ALA:HA	1:B:4276:PRO:HD3	1.92	0.40
1:C:4248:LEU:HD23	1:C:4248:LEU:HA	1.96	0.40
1:D:4666:TYR:CE1	1:D:4699:ALA:HB2	2.56	0.40
1:C:4547:PHE:HB3	1:C:4552:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/587 (99%)	566 (98%)	14 (2%)	0	100	100
1	B	563/587 (96%)	527 (94%)	36 (6%)	0	100	100
1	C	573/587 (98%)	551 (96%)	22 (4%)	0	100	100
1	D	552/587 (94%)	522 (95%)	30 (5%)	0	100	100
All	All	2268/2348 (97%)	2166 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/431 (101%)	420 (97%)	14 (3%)	34	59
1	B	424/431 (98%)	398 (94%)	26 (6%)	17	35
1	C	432/431 (100%)	420 (97%)	12 (3%)	38	64
1	D	419/431 (97%)	402 (96%)	17 (4%)	27	51
All	All	1709/1724 (99%)	1640 (96%)	69 (4%)	28	52

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4246	ARG
1	A	4300	MSE
1	A	4303	VAL
1	A	4323	LEU
1	A	4335	LYS
1	A	4371	SER
1	A	4479	LEU
1	A	4513	GLU
1	A	4593	SER
1	A	4606	ASP
1	A	4612	LEU
1	A	4626	THR
1	A	4657	THR

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Mol	Chain	Res	Type
1	A	4692	GLU
1	B	4296	MSE
1	B	4323	LEU
1	B	4335	LYS
1	B	4367	SER
1	B	4389	LEU
1	B	4413	GLU
1	B	4427	LEU
1	B	4449	GLU
1	B	4466	LYS
1	B	4469	SER
1	B	4472	GLU
1	B	4594	LEU
1	B	4598	ARG
1	B	4603	LEU
1	B	4606	ASP
1	B	4624	ASP
1	B	4654	VAL
1	B	4662	GLN
1	B	4668	CYS
1	B	4673	ARG
1	B	4694	ARG
1	B	4724	ASP
1	B	4732	HIS
1	B	4747	SER
1	B	4757	THR
1	B	4780	VAL
1	C	4323	LEU
1	C	4337	ARG
1	C	4366	SER
1	C	4371	SER
1	C	4389	LEU
1	C	4612	LEU
1	C	4622	ARG
1	C	4623	VAL
1	C	4648	VAL
1	C	4676	GLU
1	C	4756	ARG
1	C	4790	GLU
1	D	4225	GLU
1	D	4302	GLN
1	D	4335	LYS

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Mol	Chain	Res	Type
1	D	4337	ARG
1	D	4355	GLU
1	D	4366	SER
1	D	4389	LEU
1	D	4449	GLU
1	D	4494	LYS
1	D	4530	THR
1	D	4534	LEU
1	D	4548	GLN
1	D	4594	LEU
1	D	4667	VAL
1	D	4724	ASP
1	D	4760	GLU
1	D	4790	GLU

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	4587	HIS
1	A	4645	ASN
1	A	4713	HIS
1	B	4317	GLN
1	B	4348	HIS
1	B	4421	ASN
1	B	4431	GLN
1	B	4613	GLN
1	B	4645	ASN
1	C	4679	HIS
1	D	4348	HIS
1	D	4431	GLN
1	D	4645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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	$\# Z > 2$
2	NO3	C	4902	-	1,3,3	0.57	0	0,3,3	-	-
2	NO3	C	4901	-	1,3,3	0.45	0	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	574/587 (97%)	-0.49	1 (0%) 91 90	27, 43, 75, 114	2 (0%)
1	B	562/587 (95%)	-0.01	12 (2%) 63 59	34, 65, 121, 145	1 (0%)
1	C	570/587 (97%)	-0.21	6 (1%) 78 75	37, 61, 101, 144	1 (0%)
1	D	554/587 (94%)	0.12	26 (4%) 36 32	38, 69, 129, 159	0
All	All	2260/2348 (96%)	-0.15	45 (1%) 65 61	27, 59, 115, 159	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4739	PRO	5.6
1	C	4739	PRO	5.1
1	D	4778	PRO	4.3
1	B	4656	PRO	4.1
1	D	4631	PRO	3.8
1	B	4716	ALA	3.7
1	B	4661	ALA	3.5
1	C	4534	LEU	3.5
1	D	4764	ALA	3.3
1	D	4749	ALA	3.3
1	D	4751	ALA	3.2
1	D	4729	LEU	3.1
1	B	4742	LEU	3.1
1	D	4655	PRO	3.0
1	D	4654	VAL	2.9
1	B	4772	ALA	2.8
1	B	4741	VAL	2.8
1	B	4654	VAL	2.8
1	D	4669	ALA	2.7
1	D	4667	VAL	2.6
1	B	4734	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	4752	PRO	2.6
1	D	4753	ALA	2.5
1	C	4656	PRO	2.5
1	D	4718	VAL	2.5
1	C	4625	ALA	2.5
1	D	4689	LEU	2.4
1	D	4770	PRO	2.3
1	B	4762	ALA	2.3
1	B	4669	ALA	2.3
1	D	4722	VAL	2.2
1	D	4586	ARG	2.2
1	D	4780	VAL	2.2
1	C	4654	VAL	2.2
1	A	4802	ARG	2.2
1	B	4770	PRO	2.1
1	D	4728	ALA	2.1
1	C	4655	PRO	2.1
1	D	4688	PHE	2.1
1	D	4754	THR	2.1
1	B	4774	PRO	2.1
1	D	4734	ALA	2.0
1	D	4761	LEU	2.0
1	D	4776	GLY	2.0
1	D	4769	ALA	2.0

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
2	NO3	C	4901	4/4	0.84	0.14	54,57,60,69	0
2	NO3	C	4902	4/4	0.92	0.11	55,70,73,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.