Full wwPDB X-ray Structure Validation Report (i)

Oct 27, 2016 – 02:16 PM EDT

PDB ID	:	4OPE
Title	:	Streptomcyes 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

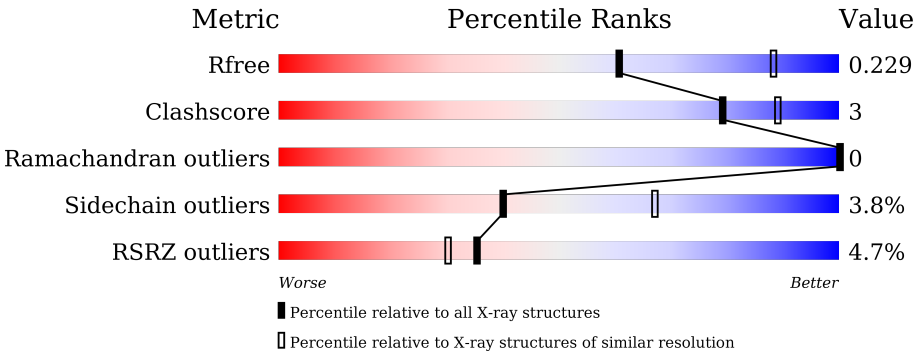
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	89% 10% •
1	B	587	6% 85% 11% • •
1	C	587	3% 86% 12% •
1	D	587	9% 83% 11% • 5%

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.

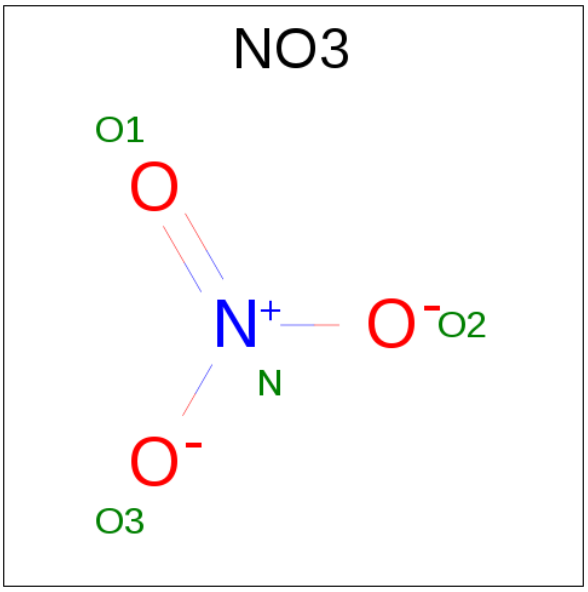
- Molecule 1 is a protein called NRPS/PKS.

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 (three-letter code: NO3) (formula: NO_3).



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

- Molecule 3 is water.

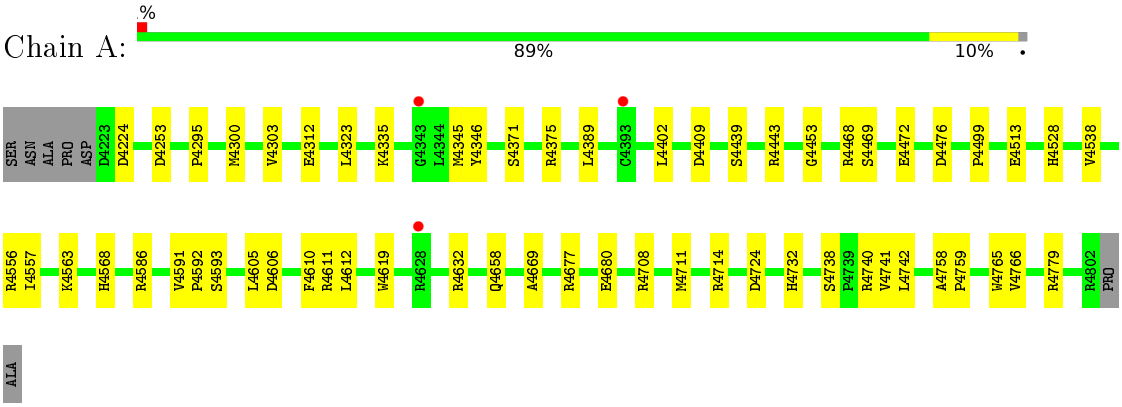
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	176	Total O 176 176	0	0
3	B	47	Total O 47 47	0	0
3	C	69	Total O 69 69	0	0
3	D	37	Total O 37 37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

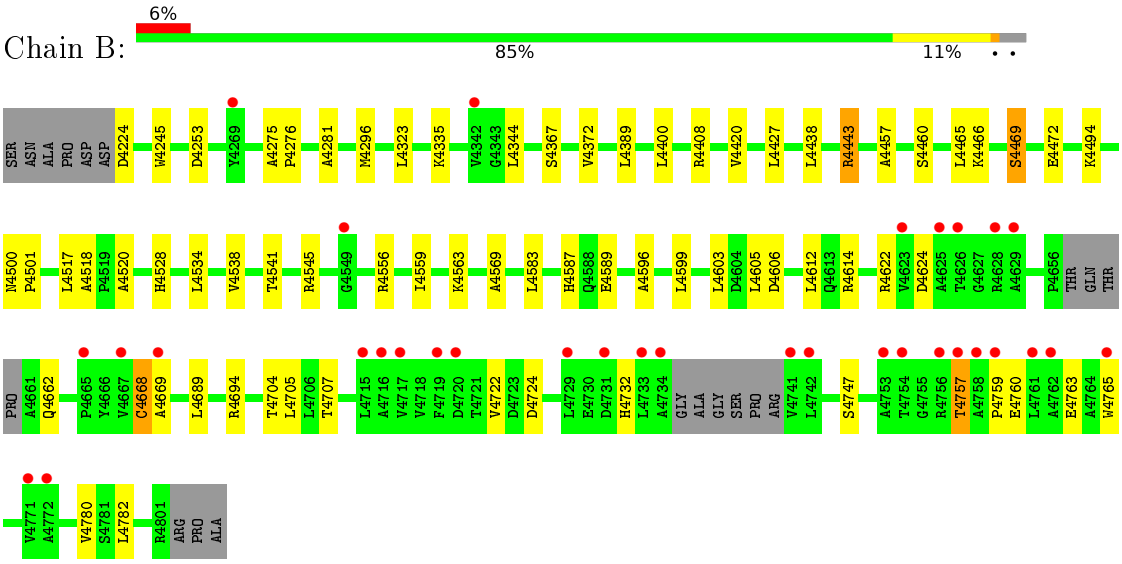
- Molecule 1: NRPS/PKS

Chain A:



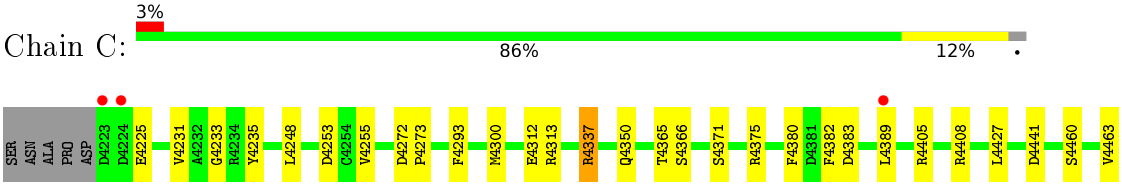
- Molecule 1: NRPS/PKS

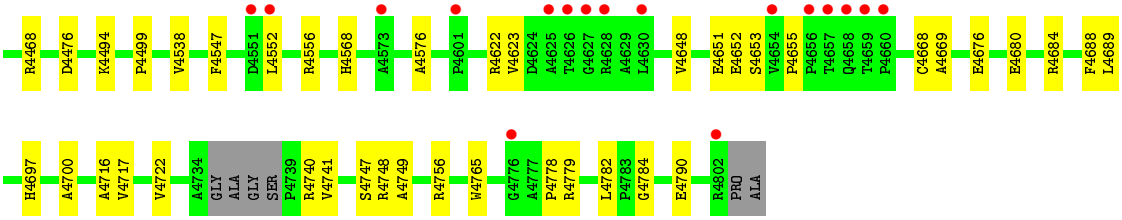
Chain B:



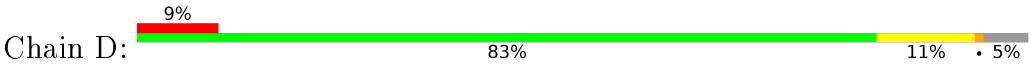
- Molecule 1: NRPS/PKS

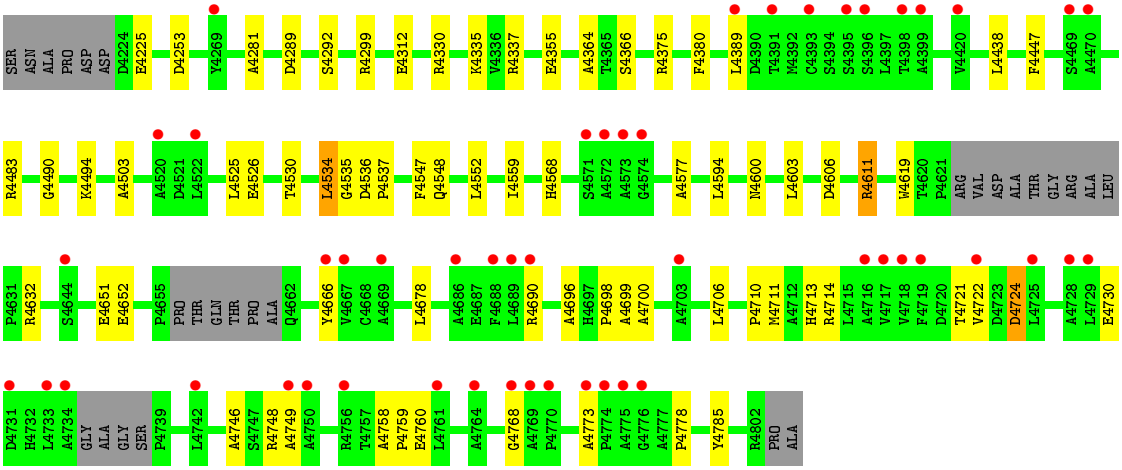
Chain C:





- Molecule 1: NRPS/PKS





4 Data and refinement statistics (i)

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 41.07 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.08-2.58) 99.6 (41.07-2.58)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.177 , 0.231 0.180 , 0.229	Depositor DCC
R_{free} test set	5179 reflections (5.28%)	DCC
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 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.75	0/4454	0.86	3/6053 (0.0%)
1	B	0.60	0/4354	0.75	2/5916 (0.0%)
1	C	0.62	0/4429	0.77	1/6019 (0.0%)
1	D	0.60	0/4298	0.74	0/5835
All	All	0.64	0/17535	0.78	6/23823 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4714	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	4708	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	4427	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	4408	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	4441	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	4611	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4257	0	4150	30	0
1	C	4329	0	4226	34	0
1	D	4205	0	4097	33	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	118	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 3.

All (118) 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:N	1:A:4658:GLN:OE1	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:D:4746:ALA:HB1	1:D:4768:GLY:HA3	1.86	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:A:4253:ASP:OD2	1:A:4443:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4668:CYS:SG	1:B:4668:CYS:O	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: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:A:4224:ASP:OD2	1:A:4469:SER:OG	2.24	0.43
1:A:4439:SER:HB3	1:A:4453:GLY:C	2.39	0.43
1:B:4732:HIS:C	1:B:4732:HIS:ND1	2.70	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: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:D:4490:GLY:HA2	1:D:4503:ALA:CB	2.49	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:B:4494:LYS:HE2	1:C:4253:ASP:CG	2.40	0.41
1:A:4738:SER:HB3	1:A:4741:VAL:HG23	2.03	0.41
1:D:4253:ASP:OD1	1:D:4253:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4559:ILE:O	1:B:4612:LEU:HA	2.21	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:4587:HIS:O	1:B:4589:GLU:HG3	2.21	0.41
1:D:4758:ALA:N	1:D:4759:PRO:HD2	2.36	0.41
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 (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	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 (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	434/431 (101%)	420 (97%)	14 (3%)	46	73
1	B	424/431 (98%)	404 (95%)	20 (5%)	32	58
1	C	432/431 (100%)	416 (96%)	16 (4%)	41	68
1	D	419/431 (97%)	403 (96%)	16 (4%)	40	67
All	All	1709/1724 (99%)	1643 (96%)	66 (4%)	40	66

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4300	MSE
1	A	4303	VAL
1	A	4323	LEU
1	A	4335	LYS
1	A	4371	SER
1	A	4409	ASP
1	A	4513	GLU
1	A	4556	ARG
1	A	4568	HIS
1	A	4593	SER
1	A	4606	ASP
1	A	4612	LEU
1	A	4677	ARG
1	A	4680	GLU
1	B	4296	MSE
1	B	4323	LEU
1	B	4335	LYS
1	B	4367	SER
1	B	4389	LEU
1	B	4443	ARG
1	B	4466	LYS
1	B	4469	SER
1	B	4472	GLU
1	B	4556	ARG
1	B	4603	LEU
1	B	4606	ASP
1	B	4624	ASP
1	B	4662	GLN
1	B	4668	CYS
1	B	4694	ARG

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Mol	Chain	Res	Type
1	B	4724	ASP
1	B	4747	SER
1	B	4757	THR
1	B	4780	VAL
1	C	4337	ARG
1	C	4366	SER
1	C	4371	SER
1	C	4389	LEU
1	C	4494	LYS
1	C	4556[A]	ARG
1	C	4556[B]	ARG
1	C	4568	HIS
1	C	4622	ARG
1	C	4623	VAL
1	C	4648	VAL
1	C	4676	GLU
1	C	4697	HIS
1	C	4740	ARG
1	C	4756	ARG
1	C	4790	GLU
1	D	4225	GLU
1	D	4299	ARG
1	D	4335	LYS
1	D	4337	ARG
1	D	4355	GLU
1	D	4366	SER
1	D	4389	LEU
1	D	4494	LYS
1	D	4530	THR
1	D	4534	LEU
1	D	4548	GLN
1	D	4568	HIS
1	D	4594	LEU
1	D	4611	ARG
1	D	4724	ASP
1	D	4760	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4587	HIS
1	A	4713	HIS

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Mol	Chain	Res	Type
1	B	4317	GLN
1	B	4348	HIS
1	D	4348	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	4901	-	1,3,3	1.08	0	0,3,3	0.00	-
2	NO3	C	4902	-	1,3,3	1.31	0	0,3,3	0.00	-

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
2	NO3	C	4901	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NO3	C	4902	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.36	3 (0%) 91 90	27, 43, 75, 114	0
1	B	562/587 (95%)	0.25	33 (5%) 26 21	34, 65, 121, 145	0
1	C	570/587 (97%)	-0.08	20 (3%) 48 42	37, 61, 101, 144	0
1	D	554/587 (94%)	0.37	50 (9%) 12 9	38, 69, 129, 159	0
All	All	2260/2348 (96%)	0.04	106 (4%) 35 30	27, 59, 115, 159	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4627	GLY	7.4
1	D	4729	LEU	7.0
1	B	4716	ALA	6.8
1	B	4734	ALA	6.0
1	C	4626	THR	5.8
1	D	4667	VAL	5.4
1	D	4669	ALA	4.9
1	D	4716	ALA	4.9
1	B	4762	ALA	4.8
1	B	4733	LEU	4.8
1	D	4725	LEU	4.8
1	B	4625	ALA	4.7
1	D	4689	LEU	4.7
1	B	4753	ALA	4.5
1	C	4657	THR	4.5
1	B	4756	ARG	4.5
1	D	4722	VAL	4.4
1	B	4629	ALA	4.2
1	B	4754	THR	4.0
1	B	4717	VAL	3.9
1	D	4776	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	4775	ALA	3.8
1	B	4626	THR	3.8
1	D	4770	PRO	3.7
1	D	4761	LEU	3.7
1	B	4759	PRO	3.6
1	C	4625	ALA	3.6
1	D	4734	ALA	3.6
1	B	4757	THR	3.4
1	D	4717	VAL	3.4
1	D	4396	SER	3.3
1	B	4741	VAL	3.3
1	B	4772	ALA	3.3
1	D	4686	ALA	3.2
1	D	4718	VAL	3.1
1	D	4764	ALA	3.1
1	D	4728	ALA	3.1
1	D	4749	ALA	3.1
1	D	4574	GLY	3.0
1	B	4761	LEU	3.0
1	C	4628	ARG	2.9
1	C	4656	PRO	2.9
1	B	4771	VAL	2.9
1	D	4733	LEU	2.9
1	D	4774	PRO	2.9
1	D	4756	ARG	2.9
1	C	4776	GLY	2.9
1	D	4703	ALA	2.9
1	B	4719	PHE	2.8
1	C	4552	LEU	2.8
1	A	4628	ARG	2.8
1	B	4269	TYR	2.7
1	D	4750	ALA	2.7
1	D	4644	SER	2.7
1	B	4628	ARG	2.7
1	C	4223	ASP	2.6
1	D	4469	SER	2.6
1	D	4768	GLY	2.6
1	D	4688	PHE	2.6
1	D	4420	VAL	2.6
1	D	4773	ALA	2.5
1	B	4667	VAL	2.5
1	B	4720	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	4395	SER	2.5
1	D	4269	TYR	2.5
1	C	4630	LEU	2.4
1	C	4659	THR	2.4
1	B	4665	PRO	2.4
1	C	4551	ASP	2.4
1	A	4393	CYS	2.4
1	B	4758	ALA	2.4
1	D	4742	LEU	2.4
1	B	4623	VAL	2.3
1	D	4731	ASP	2.3
1	B	4742	LEU	2.3
1	B	4715	LEU	2.3
1	D	4573	ALA	2.3
1	C	4802	ARG	2.3
1	C	4573	ALA	2.3
1	D	4572	ALA	2.3
1	D	4690	ARG	2.3
1	D	4391	THR	2.3
1	C	4389	LEU	2.3
1	D	4522	LEU	2.2
1	C	4224	ASP	2.2
1	B	4342	VAL	2.2
1	D	4571	SER	2.2
1	B	4549	GLY	2.2
1	B	4731	ASP	2.2
1	B	4765	TRP	2.2
1	D	4666	TYR	2.2
1	C	4658	GLN	2.1
1	D	4520	ALA	2.1
1	A	4343	GLY	2.1
1	D	4769	ALA	2.1
1	D	4719	PHE	2.1
1	B	4669	ALA	2.1
1	D	4398	THR	2.1
1	C	4660	PRO	2.1
1	B	4729	LEU	2.1
1	D	4399	ALA	2.0
1	D	4470	ALA	2.0
1	D	4389	LEU	2.0
1	D	4393	CYS	2.0
1	C	4654	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	4601	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	NO3	C	4901	4/4	0.86	0.15	1.57	54,57,60,69	0
2	NO3	C	4902	4/4	0.89	0.19	-	55,70,73,77	0

6.5 Other polymers (i)

There are no such residues in this entry.