



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 PM UTC

PDB ID : 3N0T / pdb_00003n0t
Title : Human dipeptidil peptidase DPP7 complexed with inhibitor GSK237826A
Authors : Dobrovetsky, E.; Khutoreskaya, G.; Seitova, A.; Crombet, L.; Cossar, D.; Pagannon, S.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hassell, A.; Shewchuk, L.; Haffner, C.; Bochkarev, A.; Structural Genomics Consortium (SGC)
Deposited on : 2010-05-14
Resolution : 2.45 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

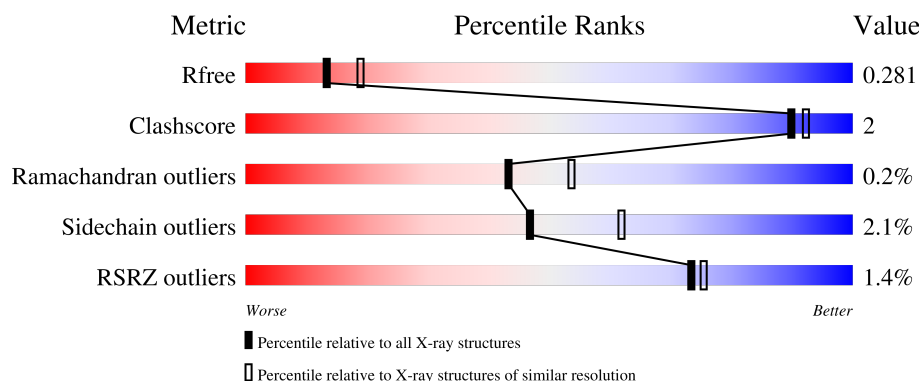
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	469	 87% 9% . .
1	B	469	 88% 8% .
1	C	469	 87% 8% .
1	D	469	 87% 8% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14133 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.

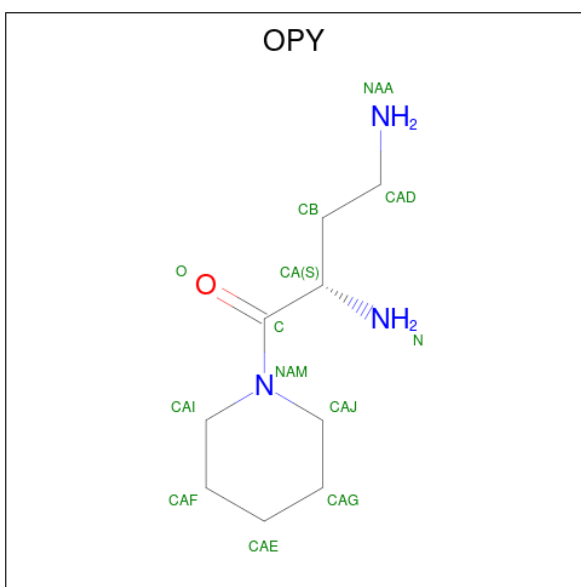
- Molecule 1 is a protein called Dipeptidyl peptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3486	2230	601	641	14			
1	B	452	Total	C	N	O	S	0	0	0
			3476	2227	597	638	14			
1	C	451	Total	C	N	O	S	0	0	0
			3449	2210	592	633	14			
1	D	449	Total	C	N	O	S	0	0	0
			3422	2194	586	628	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q9UHL4
A	25	ALA	-	expression tag	UNP Q9UHL4
A	26	MET	-	expression tag	UNP Q9UHL4
A	27	ASP	-	expression tag	UNP Q9UHL4
B	24	GLY	-	expression tag	UNP Q9UHL4
B	25	ALA	-	expression tag	UNP Q9UHL4
B	26	MET	-	expression tag	UNP Q9UHL4
B	27	ASP	-	expression tag	UNP Q9UHL4
C	24	GLY	-	expression tag	UNP Q9UHL4
C	25	ALA	-	expression tag	UNP Q9UHL4
C	26	MET	-	expression tag	UNP Q9UHL4
C	27	ASP	-	expression tag	UNP Q9UHL4
D	24	GLY	-	expression tag	UNP Q9UHL4
D	25	ALA	-	expression tag	UNP Q9UHL4
D	26	MET	-	expression tag	UNP Q9UHL4
D	27	ASP	-	expression tag	UNP Q9UHL4

- Molecule 2 is (3S)-4-oxo-4-piperidin-1-ylbutane-1,3-diamine (CCD ID: OPY) (formula: $C_9H_{19}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	3	1		
2	B	1	Total	C	N	O	0	0
			13	9	3	1		
2	C	1	Total	C	N	O	0	0
			13	9	3	1		
2	D	1	Total	C	N	O	0	0
			13	9	3	1		

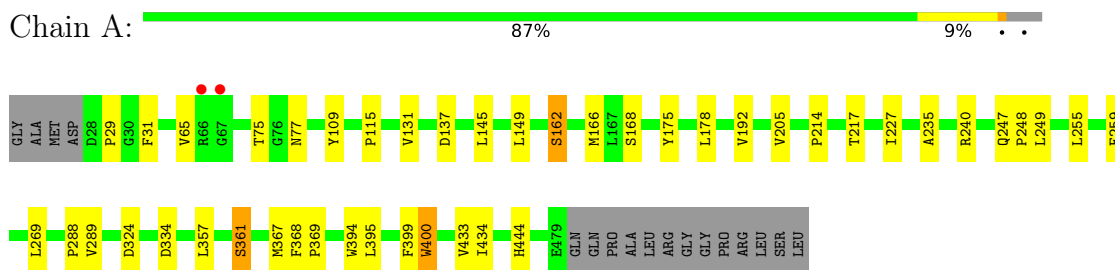
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	87	Total	O	0	0
			87	87		
3	C	41	Total	O	0	0
			41	41		
3	D	31	Total	O	0	0
			31	31		

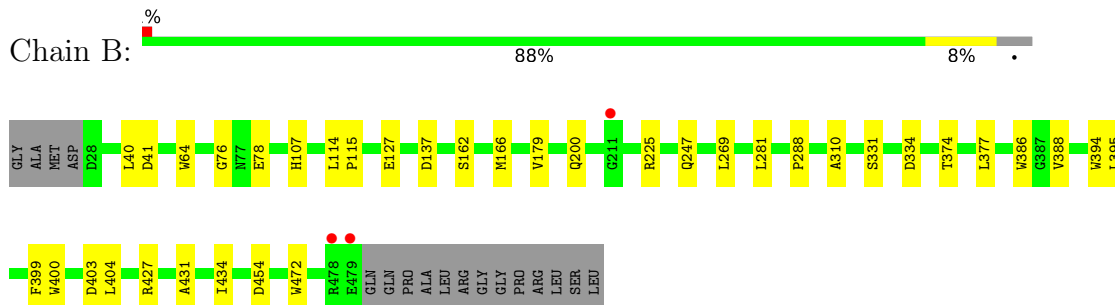
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

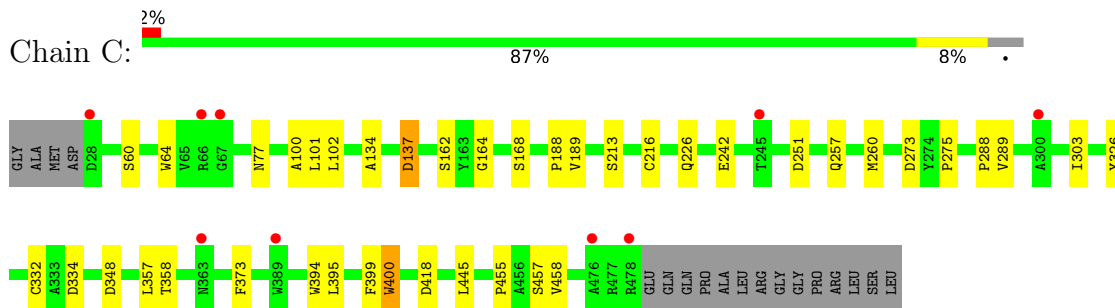
• Molecule 1: Dipeptidyl peptidase 2



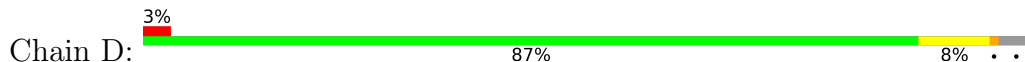
• Molecule 1: Dipeptidyl peptidase 2

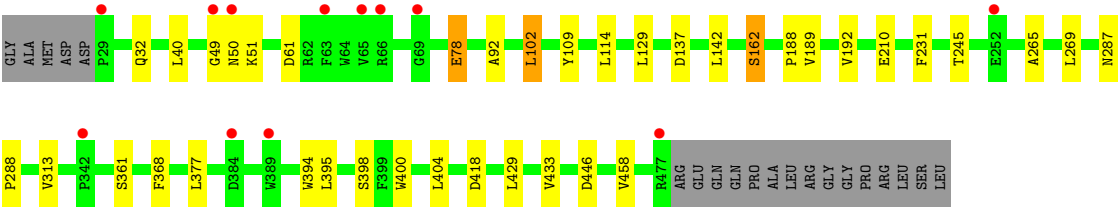


• Molecule 1: Dipeptidyl peptidase 2



• Molecule 1: Dipeptidyl peptidase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 130.50Å 125.08Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	20.01 – 2.45 20.01 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.01-2.45) 99.3 (20.01-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.47Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.218 , 0.260 0.231 , 0.281	Depositor DCC
R_{free} test set	4609 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.6	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	0.91	EDS
Total number of atoms	14133	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OPY

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	0.84	0/3584	1.39	23/4879 (0.5%)
1	B	0.86	0/3574	1.37	17/4867 (0.3%)
1	C	0.84	0/3547	1.37	19/4834 (0.4%)
1	D	0.85	1/3520 (0.0%)	1.40	15/4800 (0.3%)
All	All	0.85	1/14225 (0.0%)	1.38	74/19380 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	287	ASN	CA-CB	6.08	1.56	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	TRP	N-CA-C	7.82	119.43	111.07
1	D	394	TRP	N-CA-C	7.69	119.35	110.97
1	A	137	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	399	PHE	N-CA-C	6.94	121.05	112.59
1	D	418	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	77	ASN	N-CA-C	6.51	118.47	109.29
1	C	418	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	394	TRP	N-CA-C	6.24	118.60	111.11
1	C	399	PHE	N-CA-C	6.22	120.47	112.26
1	D	137	ASP	CA-CB-CG	6.16	118.75	112.60
1	A	399	PHE	N-CA-C	6.11	120.76	112.88
1	A	75	THR	CA-C-N	6.10	125.78	119.92
1	A	75	THR	C-N-CA	6.10	125.78	119.92
1	B	127	GLU	N-CA-C	5.82	119.20	111.75
1	A	444	HIS	N-CA-C	5.79	119.18	111.30
1	D	210	GLU	CA-C-N	5.77	126.38	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	GLU	C-N-CA	5.77	126.38	119.98
1	B	137	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	77	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	235	ALA	CA-C-N	5.62	127.81	120.28
1	A	235	ALA	C-N-CA	5.62	127.81	120.28
1	C	189	VAL	N-CA-C	5.62	117.02	110.62
1	C	137	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	472	TRP	CA-C-N	5.55	127.76	120.60
1	B	472	TRP	C-N-CA	5.55	127.76	120.60
1	A	434	ILE	N-CA-C	5.55	116.58	108.53
1	C	260	MET	CA-C-N	5.54	127.64	120.44
1	C	260	MET	C-N-CA	5.54	127.64	120.44
1	A	289	VAL	CA-C-N	5.47	127.55	120.44
1	A	289	VAL	C-N-CA	5.47	127.55	120.44
1	B	166	MET	N-CA-C	-5.47	105.22	111.07
1	C	394	TRP	N-CA-C	5.46	117.23	111.28
1	B	41	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	64	TRP	N-CA-C	5.45	118.07	109.96
1	A	433	VAL	CA-C-N	5.44	130.11	123.10
1	A	433	VAL	C-N-CA	5.44	130.11	123.10
1	D	78	GLU	CB-CG-CD	5.41	121.79	112.60
1	C	188	PRO	CA-C-N	5.40	128.15	120.53
1	C	188	PRO	C-N-CA	5.40	128.15	120.53
1	D	61	ASP	CA-C-N	5.40	128.26	120.38
1	D	61	ASP	C-N-CA	5.40	128.26	120.38
1	B	454	ASP	N-CA-C	5.39	115.79	109.60
1	C	289	VAL	N-CA-C	-5.35	105.17	111.00
1	D	433	VAL	CA-C-N	5.34	129.98	123.10
1	D	433	VAL	C-N-CA	5.34	129.98	123.10
1	B	179	VAL	N-CA-CB	5.33	118.77	111.41
1	A	227	ILE	CA-C-N	5.32	127.36	120.44
1	A	227	ILE	C-N-CA	5.32	127.36	120.44
1	A	162	SER	CB-CA-C	-5.30	110.48	116.63
1	C	251	ASP	N-CA-C	5.28	116.68	109.18
1	C	164	GLY	CA-C-N	5.27	125.80	120.00
1	C	164	GLY	C-N-CA	5.27	125.80	120.00
1	C	251	ASP	CA-C-N	5.25	127.57	120.38
1	C	251	ASP	C-N-CA	5.25	127.57	120.38
1	D	189	VAL	N-CA-C	5.24	115.97	110.62
1	A	205	VAL	N-CA-C	-5.21	105.30	110.62
1	B	200	GLN	N-CA-C	5.18	116.74	111.14
1	A	214	PRO	CA-C-N	5.15	127.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	PRO	C-N-CA	5.15	127.18	120.28
1	A	77	ASN	N-CA-C	5.14	116.53	109.29
1	D	458	VAL	CA-C-N	5.12	127.02	120.56
1	D	458	VAL	C-N-CA	5.12	127.02	120.56
1	C	242	GLU	N-CA-C	5.10	116.65	111.14
1	A	131	VAL	CA-C-N	5.10	127.07	120.44
1	A	131	VAL	C-N-CA	5.10	127.07	120.44
1	D	50	ASN	CA-C-N	5.10	131.28	121.54
1	D	50	ASN	C-N-CA	5.10	131.28	121.54
1	A	361	SER	N-CA-C	-5.05	101.63	109.72
1	C	100	ALA	N-CA-C	5.03	117.97	110.52
1	B	404	LEU	CA-C-N	5.02	127.01	120.28
1	B	404	LEU	C-N-CA	5.02	127.01	120.28
1	B	310	ALA	CA-C-N	5.02	126.42	120.14
1	B	310	ALA	C-N-CA	5.02	126.42	120.14
1	B	403	ASP	CA-CB-CG	5.02	117.62	112.60

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	3486	0	3272	15	0
1	B	3476	0	3256	8	0
1	C	3449	0	3216	16	0
1	D	3422	0	3183	9	0
2	A	13	0	19	1	0
2	B	13	0	19	2	0
2	C	13	0	19	2	0
2	D	13	0	19	1	0
3	A	89	0	0	0	0
3	B	87	0	0	0	0
3	C	41	0	0	0	0
3	D	31	0	0	0	0
All	All	14133	0	13003	48	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 2.

All (48) 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:C:162:SER:OG	2:C:1001:OPY:HAI	1.99	0.62
1:D:92:ALA:HA	1:D:102:LEU:HD21	1.84	0.60
1:A:145:LEU:O	1:A:149:LEU:HB2	2.06	0.56
1:C:162:SER:HG	2:C:1001:OPY:HAI	1.72	0.55
1:D:109:TYR:HB2	1:D:129:LEU:HD13	1.89	0.55
1:C:273:ASP:HA	1:C:288:PRO:HD2	1.91	0.53
1:A:162:SER:OG	2:A:1001:OPY:HAI	2.11	0.51
1:C:257:GLN:HE21	1:C:326:TYR:HA	1.75	0.51
1:C:332:CYS:HB2	1:C:348:ASP:OD1	2.11	0.51
1:A:247:GLN:NE2	1:A:324:ASP:OD1	2.44	0.50
1:C:334:ASP:CG	1:C:357:LEU:HD13	2.36	0.50
1:D:404:LEU:HB2	1:D:429:LEU:HD13	1.94	0.49
1:A:255:LEU:HD11	1:A:259:PHE:CZ	2.48	0.49
1:C:358:THR:HA	1:C:373:PHE:HD2	1.79	0.48
1:D:269:LEU:HD22	1:D:288:PRO:HB2	1.95	0.48
1:C:134:ALA:O	1:C:137:ASP:HB2	2.13	0.47
1:D:162:SER:OG	2:D:1001:OPY:HAI	2.15	0.47
1:B:162:SER:OG	2:B:1001:OPY:HAI	2.15	0.47
1:B:269:LEU:HD22	1:B:288:PRO:HB2	1.97	0.47
1:A:109:TYR:CE2	1:A:115:PRO:HG2	2.50	0.46
1:A:166:MET:HE3	1:A:192:VAL:HG21	1.96	0.46
1:B:386:TRP:HB2	1:B:388:VAL:HG22	1.97	0.46
1:A:217:THR:HG22	1:A:367:MET:SD	2.57	0.45
1:C:400:TRP:CD1	1:C:400:TRP:N	2.83	0.45
1:A:29:PRO:HG2	1:A:31:PHE:CE2	2.52	0.44
1:B:374:THR:H	1:B:377:LEU:HD12	1.82	0.44
1:A:269:LEU:HD22	1:A:288:PRO:HB2	1.99	0.44
1:D:361:SER:HB2	1:D:368:PHE:HB2	2.00	0.43
1:B:431:ALA:O	1:B:434:ILE:HD11	2.19	0.43
1:A:400:TRP:CD1	1:A:400:TRP:N	2.86	0.43
1:C:60:SER:HB3	1:C:102:LEU:HB2	2.01	0.43
1:D:446:ASP:N	1:D:446:ASP:OD1	2.52	0.42
1:C:213:SER:HB3	1:C:216:CYS:HB2	2.01	0.42
1:C:358:THR:HA	1:C:373:PHE:CD2	2.54	0.42
1:B:114:LEU:HA	1:B:115:PRO:HD3	1.94	0.42
1:B:334:ASP:OD2	2:B:1001:OPY:HA	2.18	0.42
1:C:445:LEU:HG	1:C:458:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASP:CG	1:A:357:LEU:HD13	2.45	0.42
1:A:259:PHE:CG	1:A:369:PRO:HG2	2.55	0.41
1:C:226:GLN:HB3	1:C:303:ILE:HD11	2.02	0.41
1:B:76:GLY:O	1:B:107:HIS:HB2	2.20	0.41
1:C:275:PRO:HG3	1:C:455:PRO:HD3	2.02	0.41
1:A:175:TYR:HB3	1:A:178:LEU:HD12	2.03	0.41
1:D:265:ALA:HA	1:D:313:VAL:HG21	2.03	0.41
1:D:188:PRO:O	1:D:192:VAL:HG22	2.21	0.41
1:A:361:SER:HB2	1:A:368:PHE:HB2	2.03	0.41
1:C:64:TRP:CG	1:C:101:LEU:HB2	2.56	0.41
1:A:240:ARG:HD2	1:A:248:PRO:HA	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	450/469 (96%)	427 (95%)	23 (5%)	0	100	100
1	B	450/469 (96%)	431 (96%)	18 (4%)	1 (0%)	43	54
1	C	449/469 (96%)	419 (93%)	30 (7%)	0	100	100
1	D	447/469 (95%)	421 (94%)	23 (5%)	3 (1%)	18	24
All	All	1796/1876 (96%)	1698 (94%)	94 (5%)	4 (0%)	43	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	51	LYS
1	B	78	GLU
1	D	49	GLY
1	D	78	GLU

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	343/371 (92%)	338 (98%)	5 (2%)	57	70
1	B	339/371 (91%)	331 (98%)	8 (2%)	43	58
1	C	335/371 (90%)	331 (99%)	4 (1%)	63	74
1	D	332/371 (90%)	320 (96%)	12 (4%)	31	45
All	All	1349/1484 (91%)	1320 (98%)	29 (2%)	47	62

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	168	SER
1	A	249	LEU
1	A	395	LEU
1	A	400	TRP
1	B	40	LEU
1	B	225	ARG
1	B	247	GLN
1	B	281	LEU
1	B	331	SER
1	B	395	LEU
1	B	400	TRP
1	B	427	ARG
1	C	168	SER
1	C	395	LEU
1	C	400	TRP
1	C	457	SER
1	D	32	GLN
1	D	40	LEU
1	D	102	LEU
1	D	114	LEU
1	D	142	LEU
1	D	162	SER
1	D	231	PHE

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Mol	Chain	Res	Type
1	D	245	THR
1	D	377	LEU
1	D	395	LEU
1	D	398	SER
1	D	400	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	86	ASN
1	A	125	HIS
1	A	226	GLN
1	A	257	GLN
1	B	125	HIS
1	C	32	GLN
1	C	122	GLN
1	C	212	GLN
1	C	264	ASN
1	C	350	GLN
1	C	439	GLN
1	D	38	GLN
1	D	86	ASN
1	D	350	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	OPY	B	1001	-	13,13,13	0.73	0	15,16,16	1.27	2 (13%)
2	OPY	C	1001	-	13,13,13	0.82	0	15,16,16	1.37	2 (13%)
2	OPY	D	1001	-	13,13,13	0.75	0	15,16,16	1.31	1 (6%)
2	OPY	A	1001	-	13,13,13	0.72	0	15,16,16	1.27	3 (20%)

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	OPY	B	1001	-	-	2/11/19/19	0/1/1/1
2	OPY	C	1001	-	-	0/11/19/19	0/1/1/1
2	OPY	D	1001	-	-	0/11/19/19	0/1/1/1
2	OPY	A	1001	-	-	0/11/19/19	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	OPY	CAJ-NAM-CAI	3.84	120.51	112.68
2	C	1001	OPY	CAJ-NAM-CAI	3.44	119.70	112.68
2	B	1001	OPY	CAJ-NAM-CAI	3.25	119.31	112.68
2	A	1001	OPY	CAJ-NAM-CAI	2.73	118.24	112.68
2	A	1001	OPY	CA-C-NAM	2.61	122.78	118.85
2	A	1001	OPY	O-C-NAM	-2.40	118.75	121.61
2	C	1001	OPY	O-C-NAM	-2.27	118.90	121.61
2	B	1001	OPY	CA-C-NAM	2.18	122.14	118.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	OPY	O-C-CA-N
2	B	1001	OPY	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	OPY	2	0
2	C	1001	OPY	2	0
2	D	1001	OPY	1	0
2	A	1001	OPY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	452/469 (96%)	-0.12	2 (0%) 88 89	22, 33, 52, 66	0
1	B	452/469 (96%)	-0.09	3 (0%) 84 86	23, 33, 49, 79	0
1	C	451/469 (96%)	0.34	9 (1%) 65 66	31, 46, 64, 79	0
1	D	449/469 (95%)	0.38	12 (2%) 56 57	30, 47, 65, 77	0
All	All	1804/1876 (96%)	0.13	26 (1%) 73 75	22, 41, 60, 79	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	PRO	3.8
1	D	66	ARG	3.4
1	C	28	ASP	2.8
1	C	478	ARG	2.8
1	C	67	GLY	2.7
1	C	300	ALA	2.7
1	B	479	GLU	2.6
1	D	477	ARG	2.6
1	D	252	GLU	2.6
1	C	389	TRP	2.5
1	D	49	GLY	2.4
1	C	476	ALA	2.3
1	D	69	GLY	2.3
1	D	342	PRO	2.2
1	A	66	ARG	2.2
1	D	63	PHE	2.2
1	C	245	THR	2.1
1	C	66	ARG	2.1
1	D	50	ASN	2.1
1	D	384	ASP	2.1
1	D	65	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	363	ASN	2.1
1	B	211	GLY	2.1
1	D	389	TRP	2.1
1	A	67	GLY	2.1
1	B	478	ARG	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
2	OPY	A	1001	13/13	0.93	0.08	20,25,43,43	0
2	OPY	C	1001	13/13	0.94	0.09	19,38,71,78	0
2	OPY	D	1001	13/13	0.94	0.08	24,32,66,76	0
2	OPY	B	1001	13/13	0.96	0.07	9,26,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.