



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:08 pm GMT

PDB ID : 3G0C
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 1
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.
Deposited on : 2009-01-27
Resolution : 2.69 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

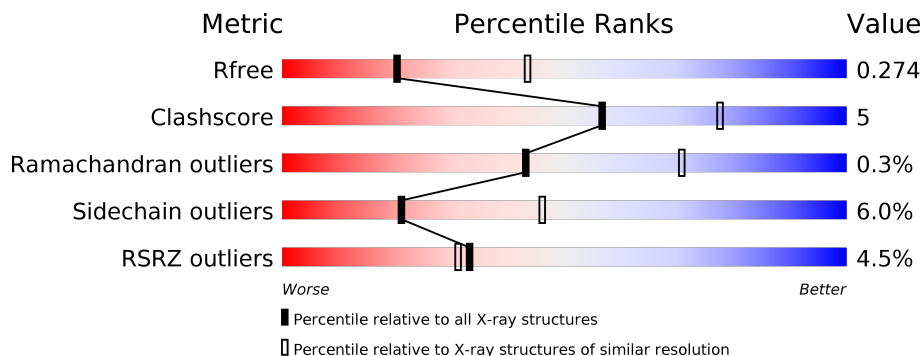
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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 $\leq 5\%$. 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	740	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	740	<div> <div></div> <div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	740	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	740	<div> <div>10%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24940 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	1	0
			5920	3804	972	1118	26			
1	B	729	Total	C	N	O	S	0	1	0
			5972	3834	986	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5929	3809	974	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

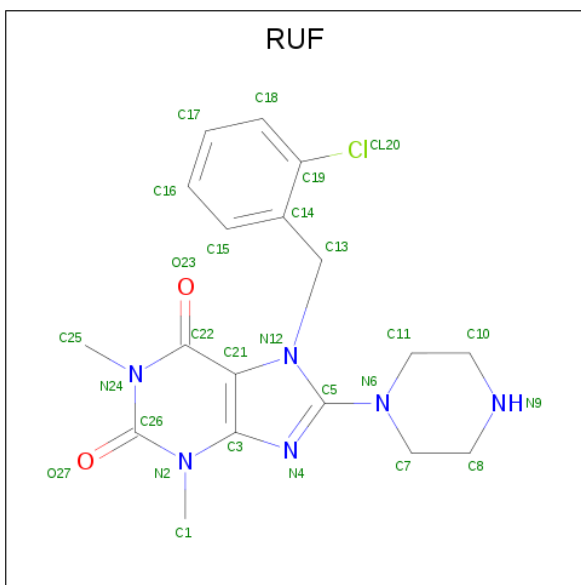
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

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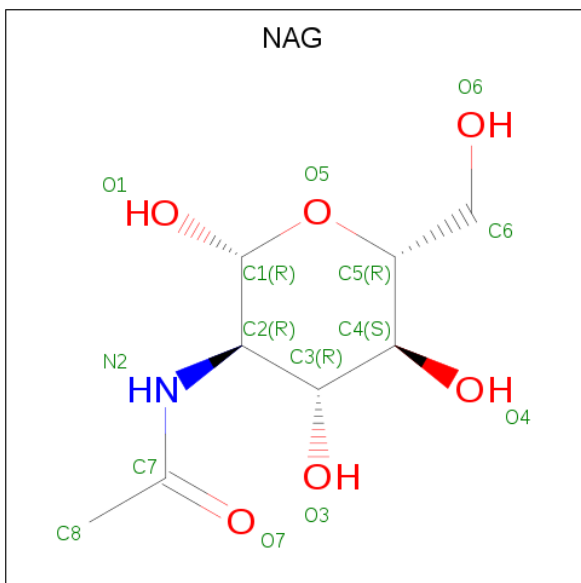
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 7-(2-chlorobenzyl)-1,3-dimethyl-8-piperazin-1-yl-3,7-dihydro-1H-purine-2,6-dione (three-letter code: RUF) (formula: C₁₈H₂₁ClN₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

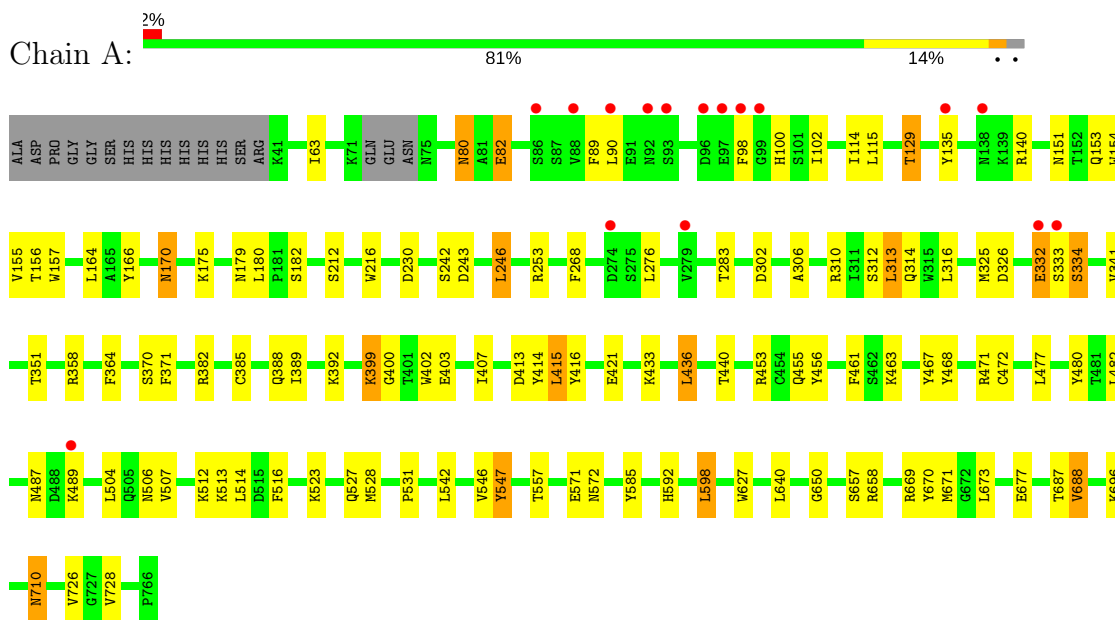
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	231	Total 231	O 231	0	0
4	B	237	Total 237	O 237	0	0
4	C	196	Total 196	O 196	0	0
4	D	110	Total 110	O 110	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 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.

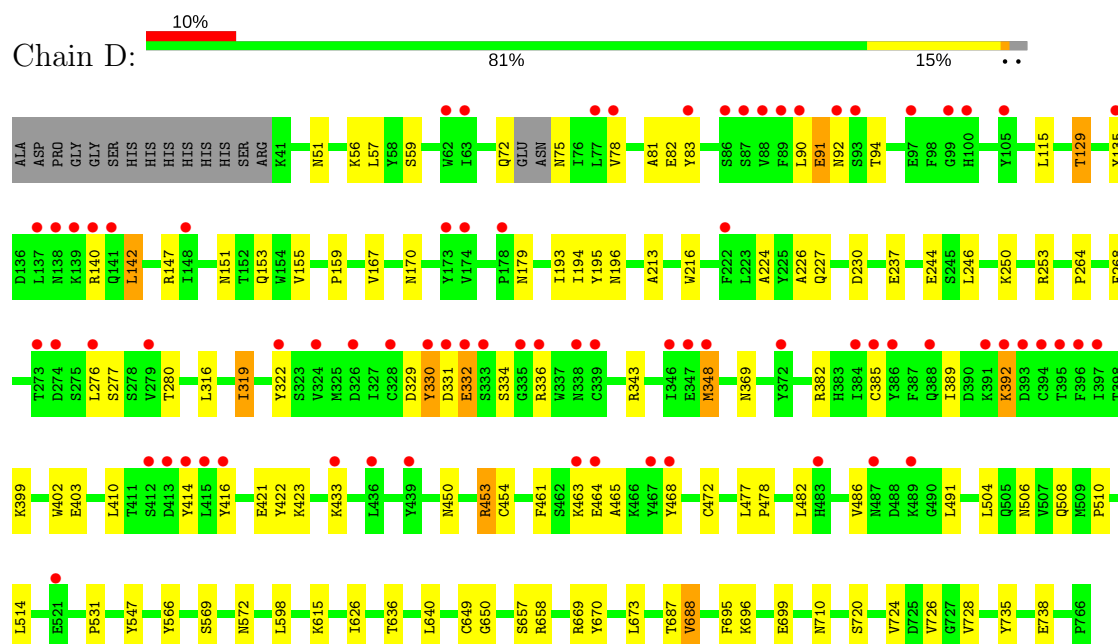
• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.84Å 122.77Å 145.11Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 48.57 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.69) 99.2 (48.57-2.69)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.248 0.236 , 0.274	Depositor DCC
R_{free} test set	5412 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24940	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: RUF, NAG

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	0.46	0/6091	0.61	0/8284
1	B	0.47	0/6149	0.61	1/8362 (0.0%)
1	C	0.46	0/6100	0.61	0/8296
1	D	0.50	4/6100 (0.1%)	0.59	1/8296 (0.0%)
All	All	0.47	4/24440 (0.0%)	0.61	2/33238 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	GLU	CD-OE1	9.06	1.35	1.25
1	D	332	GLU	CD-OE2	8.97	1.35	1.25
1	D	330	TYR	CE1-CZ	5.96	1.46	1.38
1	D	330	TYR	CG-CD2	5.90	1.46	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	415	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5920	0	5638	65	0
1	B	5972	0	5681	75	0
1	C	5929	0	5649	52	0
1	D	5929	0	5650	55	0
2	A	27	0	21	2	0
2	B	27	0	21	2	0
2	C	27	0	21	4	0
2	D	27	0	21	2	0
3	A	112	0	102	0	0
3	B	84	0	77	0	0
3	C	56	0	51	0	0
3	D	56	0	51	1	0
4	A	231	0	0	3	0
4	B	237	0	0	4	0
4	C	196	0	0	2	0
4	D	110	0	0	1	0
All	All	24940	0	22983	253	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 5.

All (253) 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:153:GLN:HE22	1:A:170:ASN:H	1.15	0.91
1:C:153:GLN:HE22	1:C:170:ASN:H	1.10	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.15	0.90
1:D:90:LEU:HD12	1:D:140:ARG:HH21	1.39	0.87
1:C:54:ARG:HH21	1:C:54:ARG:HG2	1.41	0.86
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.79
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.66	0.77
1:D:277:SER:HB3	1:D:280:THR:HG22	1.70	0.73
1:B:78:VAL:HG22	1:B:89:PHE:HB2	1.70	0.73
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.72	0.72
1:B:391:LYS:HE3	1:B:391:LYS:HA	1.73	0.69
1:D:153:GLN:HE22	1:D:170:ASN:H	1.38	0.69
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.91	0.69
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.75	0.68
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.30	0.67
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.76	0.65
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.78	0.65
1:B:36:HIS:CD2	1:B:37:HIS:H	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASN:OD1	1:B:340:LEU:HD12	1.97	0.64
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.80	0.63
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.79	0.63
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.81	0.62
1:B:98:PHE:HE1	1:B:100:HIS:HB2	1.64	0.62
1:B:179:ASN:H	1:B:179:ASN:HD22	1.45	0.61
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.65	0.61
1:A:399:LYS:HD2	1:A:400:GLY:N	2.16	0.61
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.82	0.60
1:A:358[A]:ARG:HD2	4:A:903:HOH:O	2.01	0.60
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.84	0.60
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.83	0.60
1:D:450:ASN:O	1:D:454:CYS:HB2	2.03	0.59
1:B:391:LYS:HD3	1:B:392:LYS:H	1.68	0.58
1:A:546:VAL:HG12	1:A:627:TRP:O	2.03	0.57
1:A:170:ASN:N	1:A:170:ASN:HD22	2.02	0.57
1:D:129:THR:HG23	1:D:151:ASN:HA	1.85	0.57
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.85	0.57
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.86	0.57
1:C:129:THR:HG23	1:C:151:ASN:HA	1.85	0.57
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.39	0.57
1:D:422:TYR:CE1	1:D:423:LYS:HE2	2.40	0.57
1:D:461:PHE:CD2	1:D:465:ALA:HB1	2.40	0.57
1:A:129:THR:HG23	1:A:151:ASN:HA	1.86	0.57
1:C:531:PRO:HB3	1:C:572:ASN:ND2	2.20	0.56
1:B:334:SER:HB3	1:B:336:ARG:HG3	1.87	0.56
1:D:72:GLN:HB2	1:D:75:ASN:HB2	1.87	0.56
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.87	0.56
2:A:800:RUF:C13	2:A:800:RUF:H11	2.36	0.56
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.55
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.18	0.55
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.89	0.54
1:B:283:THR:HG22	4:B:849:HOH:O	2.07	0.54
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.89	0.54
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.42	0.54
1:B:41:LYS:HE2	1:B:506:ASN:HB3	1.90	0.54
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.42	0.54
2:C:800:RUF:H11	2:C:800:RUF:H13A	1.90	0.54
2:A:800:RUF:H13A	2:A:800:RUF:H11	1.88	0.54
1:A:487:ASN:OD1	1:A:489:LYS:HG2	2.08	0.54
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.53
2:C:800:RUF:H11	2:C:800:RUF:C13	2.37	0.53
1:A:399:LYS:HD2	1:A:400:GLY:H	1.73	0.53
1:C:54:ARG:NH2	1:C:54:ARG:HG2	2.17	0.53
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.92	0.53
1:A:477:LEU:HD12	1:A:477:LEU:H	1.73	0.53
1:D:147:ARG:HE	3:D:801:NAG:H83	1.73	0.53
1:C:535:ASP:HB3	1:C:538:LYS:HG3	1.90	0.52
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.91	0.52
1:D:330:TYR:CE2	1:D:332:GLU:HA	2.44	0.52
1:A:407:ILE:HG23	1:A:415:LEU:CD1	2.38	0.52
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.90	0.52
1:B:657:SER:HA	1:B:688:VAL:HG13	1.90	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.45	0.51
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.75	0.51
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.93	0.51
2:B:800:RUF:H15	2:B:800:RUF:C21	2.40	0.51
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.75	0.51
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.91	0.51
1:B:72:GLN:HB2	1:B:75:ASN:HB2	1.93	0.51
1:C:505:GLN:HG2	4:C:849:HOH:O	2.10	0.51
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.75	0.51
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.92	0.51
1:B:608:GLU:O	1:B:612:GLN:HG2	2.11	0.51
1:C:410:LEU:HD22	1:C:411:THR:O	2.11	0.50
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.93	0.50
1:D:657:SER:HA	1:D:688:VAL:HG13	1.93	0.50
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.93	0.50
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.12	0.50
2:D:800:RUF:C13	2:D:800:RUF:H11	2.42	0.50
1:C:172:ILE:HG22	1:C:185:ILE:HD12	1.94	0.50
1:C:129:THR:HG22	4:C:777:HOH:O	2.11	0.50
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.93	0.50
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.94	0.50
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.93	0.49
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.49
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.13	0.49
1:D:508:GLN:HG2	4:D:823:HOH:O	2.12	0.49
1:D:695:PHE:HB3	1:D:728:VAL:HG11	1.95	0.49
1:D:382:ARG:H	1:D:403:GLU:HG2	1.76	0.49
1:D:91:GLU:HB3	1:D:94:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.95	0.49
1:C:145:GLU:HG2	1:C:146:GLU:HG2	1.95	0.49
1:C:453:ARG:NH2	1:C:477:LEU:O	2.41	0.49
1:A:407:ILE:HG23	1:A:415:LEU:HD11	1.94	0.48
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.77	0.48
1:D:322:TYR:HA	1:D:348:MET:HB3	1.95	0.48
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.94	0.48
1:A:333:SER:O	1:A:334:SER:HB3	2.13	0.48
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.78	0.48
1:A:80:ASN:HD22	1:A:82:GLU:H	1.61	0.48
1:B:135:TYR:CE1	1:B:141:GLN:HA	2.49	0.48
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.78	0.48
1:A:415:LEU:HD12	1:A:416:TYR:N	2.27	0.48
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.49	0.48
1:C:315:TRP:O	1:C:323:SER:HB2	2.14	0.48
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.96	0.48
1:D:75:ASN:HA	1:D:91:GLU:HG3	1.96	0.48
1:A:332:GLU:HA	1:A:332:GLU:OE2	2.14	0.48
2:D:800:RUF:H11	2:D:800:RUF:C14	2.44	0.47
1:A:82:GLU:OE1	1:A:82:GLU:HA	2.14	0.47
1:B:471[A]:ARG:HG3	1:B:480:TYR:CE1	2.50	0.47
1:B:635:VAL:O	1:B:639:VAL:HG23	2.14	0.47
1:D:392:LYS:HD2	1:D:392:LYS:H	1.79	0.47
1:C:504:LEU:HA	1:C:507:VAL:HG13	1.96	0.47
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.79	0.47
1:C:517:ILE:HD13	1:C:612:GLN:HG3	1.97	0.47
1:D:461:PHE:CE2	1:D:468:TYR:HB3	2.49	0.47
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.15	0.47
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.45	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.46
1:D:135:TYR:CZ	1:D:142:LEU:HB2	2.50	0.46
1:D:369:ASN:O	1:D:389:ILE:HG12	2.16	0.46
1:D:91:GLU:HB3	1:D:94:THR:N	2.30	0.46
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.50	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.46
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.50	0.46
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.80	0.46
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.51	0.46
1:A:657:SER:HA	1:A:688:VAL:HG13	1.97	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.97	0.46
1:D:657:SER:HA	1:D:688:VAL:CG1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PRO:HG2	1:B:158:SER:O	2.15	0.46
1:D:115:LEU:HD21	1:D:155:VAL:HG21	1.98	0.46
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.31	0.46
1:A:102:ILE:H	1:A:102:ILE:HD12	1.80	0.46
1:A:306:ALA:HB3	1:A:310:ARG:HG2	1.98	0.46
1:B:129:THR:HG22	4:B:890:HOH:O	2.16	0.46
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.98	0.45
1:B:242:SER:OG	1:B:243:ASP:N	2.47	0.45
1:A:312:SER:HA	1:A:326:ASP:O	2.17	0.45
2:B:800:RUF:C14	2:B:800:RUF:H11	2.46	0.45
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.97	0.45
1:B:491:LEU:O	1:B:492:ARG:HB3	2.17	0.45
1:D:319:ILE:HG13	1:D:319:ILE:H	1.55	0.45
1:D:81:ALA:C	1:D:83:TYR:H	2.19	0.45
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.46	0.45
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.82	0.45
1:B:170:ASN:N	1:B:170:ASN:HD22	2.14	0.45
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.52	0.45
1:D:343:ARG:HG2	1:D:389:ILE:HG22	1.99	0.45
1:A:571:GLU:HA	1:A:571:GLU:OE2	2.16	0.45
1:B:56:LYS:HE3	1:B:495:GLU:OE2	2.17	0.45
1:A:710:ASN:C	1:A:710:ASN:HD22	2.21	0.44
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.98	0.44
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.00	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.44
1:D:213:ALA:HB1	1:D:226:ALA:HB3	1.99	0.44
1:A:388:GLN:NE2	4:A:974:HOH:O	2.50	0.44
1:C:109:PRO:HG2	1:C:158:SER:O	2.18	0.44
1:D:640:LEU:HD11	1:D:650:GLY:HA3	2.00	0.44
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.99	0.44
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.98	0.43
1:A:414:TYR:CD2	1:A:433:LYS:HD3	2.53	0.43
1:A:115:LEU:HD21	1:A:155:VAL:HG21	2.00	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.43
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.33	0.43
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.19	0.43
1:B:92:ASN:ND2	4:B:980:HOH:O	2.51	0.43
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.18	0.43
1:A:89:PHE:O	1:A:90:LEU:HG	2.19	0.43
1:B:167:VAL:HG11	1:B:198:ILE:HG12	2.01	0.43
1:B:127:SER:HB3	1:B:211:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:ND2	1:B:299:TYR:OH	2.51	0.43
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.53	0.43
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.54	0.43
1:D:720:SER:O	1:D:724:VAL:HG23	2.19	0.43
1:C:657:SER:HA	1:C:688:VAL:HG13	2.00	0.43
1:A:382:ARG:NH2	4:A:1:HOH:O	2.52	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.53	0.42
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.49	0.42
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.54	0.42
1:B:72:GLN:HG3	1:B:77:LEU:CD2	2.50	0.42
1:D:416:TYR:CE1	1:D:433:LYS:HE2	2.55	0.42
1:B:167:VAL:HA	1:B:171:ASP:O	2.20	0.42
1:B:306:ALA:HB3	1:B:310:ARG:HG2	2.01	0.42
1:C:710:ASN:C	1:C:710:ASN:HD22	2.23	0.42
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.50	0.42
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.54	0.42
1:A:175:LYS:NZ	1:A:180:LEU:O	2.43	0.42
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.19	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.55	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.02	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:D:453:ARG:NH2	1:D:477:LEU:O	2.49	0.42
1:C:42:THR:HG22	1:C:508:GLN:HG3	2.02	0.42
1:C:516:PHE:CG	1:C:523:LYS:HE3	2.54	0.42
1:D:195:TYR:O	1:D:227:GLN:HA	2.20	0.42
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.55	0.42
1:B:54:ARG:HG3	4:B:884:HOH:O	2.20	0.42
1:B:95:PHE:HE1	1:B:135:TYR:CD1	2.37	0.42
1:C:388:GLN:HB2	1:C:391:LYS:HG2	2.02	0.42
1:D:626:ILE:HG23	1:D:636:THR:HG23	2.01	0.42
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.20	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.20	0.41
1:A:325:MET:CE	1:A:371:PHE:CZ	3.03	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.19	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.41
1:D:735:TYR:HB3	1:D:738:GLU:HG3	2.02	0.41
1:C:387:PHE:CD1	1:C:394:CYS:HB3	2.55	0.41
1:C:726:VAL:HG23	1:C:728:VAL:HG23	2.01	0.41
1:B:36:HIS:CG	1:B:37:HIS:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASN:C	1:C:389:ILE:HG12	2.41	0.41
1:C:405:ILE:HB	1:C:418:ILE:HG22	2.01	0.41
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.55	0.41
1:B:688:VAL:HG22	1:B:719:ILE:HG12	2.01	0.41
1:B:744:SER:HB2	1:B:747:ALA:HB3	2.03	0.41
1:C:711:VAL:HG23	2:C:800:RUF:H17	2.02	0.41
1:A:547:TYR:CD1	1:A:547:TYR:C	2.94	0.41
1:C:666:TYR:CD1	2:C:800:RUF:H11A	2.56	0.41
1:C:123:GLN:HB3	1:C:127:SER:OG	2.20	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	0.41
1:C:79:PHE:CE2	1:C:86:SER:HB3	2.56	0.41
1:B:506:ASN:HA	1:B:506:ASN:HD22	1.60	0.41
1:B:547:TYR:CD1	1:B:547:TYR:C	2.94	0.41
1:C:547:TYR:C	1:C:547:TYR:CD1	2.94	0.41
1:D:153:GLN:NE2	1:D:167:VAL:HG12	2.36	0.41
1:C:162:HIS:NE2	1:C:177:GLU:OE1	2.54	0.40
1:C:602:GLU:OE1	1:C:602:GLU:N	2.51	0.40
1:D:726:VAL:HG23	1:D:728:VAL:HG23	2.03	0.40
1:B:164:LEU:HB3	1:B:175:LYS:HB2	2.04	0.40
1:B:326:ASP:OD2	1:B:344:GLN:HG3	2.21	0.40
1:B:474:GLY:HA2	1:B:476:GLY:O	2.21	0.40
1:C:492:ARG:NH2	1:C:492:ARG:HB3	2.37	0.40
1:D:510:PRO:HD3	1:D:569:SER:HB2	2.03	0.40
1:A:512:LYS:HA	1:A:528:MET:O	2.21	0.40
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.03	0.40
1:A:155:VAL:HG12	1:A:166:TYR:HB3	2.02	0.40
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.56	0.40
1:B:751:ILE:O	1:B:755:MET:HG3	2.21	0.40
1:C:195:TYR:O	1:C:227:GLN:HA	2.21	0.40
1:C:658:ARG:HG3	1:C:687:THR:HG22	2.03	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	719/740 (97%)	684 (95%)	31 (4%)	4 (1%)	27	54
1	B	726/740 (98%)	698 (96%)	27 (4%)	1 (0%)	53	80
1	C	720/740 (97%)	679 (94%)	39 (5%)	2 (0%)	43	71
1	D	720/740 (97%)	664 (92%)	55 (8%)	1 (0%)	53	80
All	All	2885/2960 (98%)	2725 (94%)	152 (5%)	8 (0%)	43	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
1	A	140	ARG
1	A	334	SER
1	A	463	LYS
1	C	423	LYS
1	C	334	SER
1	D	244	GLU
1	B	742	ILE

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	648/662 (98%)	611 (94%)	37 (6%)	23	48
1	B	653/662 (99%)	607 (93%)	46 (7%)	16	38
1	C	649/662 (98%)	612 (94%)	37 (6%)	23	48
1	D	649/662 (98%)	613 (94%)	36 (6%)	24	50
All	All	2599/2648 (98%)	2443 (94%)	156 (6%)	21	46

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	80	ASN
1	A	82	GLU
1	A	129	THR
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	230	ASP
1	A	243	ASP
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	341	VAL
1	A	370	SER
1	A	385	CYS
1	A	392	LYS
1	A	399	LYS
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	453	ARG
1	A	472	CYS
1	A	482	LEU
1	A	504	LEU
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	542	LEU
1	A	547	TYR
1	A	598	LEU
1	A	673	LEU
1	A	677	GLU
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	46	THR
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	72	GLN

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Mol	Chain	Res	Type
1	B	78	VAL
1	B	82	GLU
1	B	129	THR
1	B	170	ASN
1	B	179	ASN
1	B	246	LEU
1	B	276	LEU
1	B	295	ILE
1	B	316	LEU
1	B	326	ASP
1	B	336	ARG
1	B	343	ARG
1	B	344	GLN
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	472	CYS
1	B	482	LEU
1	B	492	ARG
1	B	504	LEU
1	B	506	ASN
1	B	514	LEU
1	B	515	ASP
1	B	538	LYS
1	B	547	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	614	SER
1	B	660	GLU
1	B	673	LEU
1	B	688	VAL
1	B	704	HIS
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU

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Mol	Chain	Res	Type
1	C	72	GLN
1	C	75	ASN
1	C	87	SER
1	C	129	THR
1	C	145	GLU
1	C	243	ASP
1	C	246	LEU
1	C	283	THR
1	C	316	LEU
1	C	339	CYS
1	C	366	LEU
1	C	378	GLU
1	C	379	GLU
1	C	385	CYS
1	C	390	ASP
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	441	LYS
1	C	453	ARG
1	C	460	SER
1	C	463	LYS
1	C	482	LEU
1	C	492	ARG
1	C	496	ASP
1	C	504	LEU
1	C	507	VAL
1	C	519	LEU
1	C	546	VAL
1	C	547	TYR
1	C	566	TYR
1	C	630	SER
1	C	673	LEU
1	C	710	ASN
1	C	761	GLN
1	D	51	ASN
1	D	56	LYS
1	D	57	LEU
1	D	59	SER
1	D	78	VAL
1	D	82	GLU
1	D	91	GLU

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Mol	Chain	Res	Type
1	D	92	ASN
1	D	129	THR
1	D	179	ASN
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	316	LEU
1	D	319	ILE
1	D	329	ASP
1	D	336	ARG
1	D	348	MET
1	D	385	CYS
1	D	392	LYS
1	D	399	LYS
1	D	410	LEU
1	D	453	ARG
1	D	463	LYS
1	D	464	GLU
1	D	486	VAL
1	D	504	LEU
1	D	506	ASN
1	D	514	LEU
1	D	547	TYR
1	D	566	TYR
1	D	598	LEU
1	D	615	LYS
1	D	673	LEU
1	D	688	VAL
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	80	ASN
1	A	138	ASN
1	A	151	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN

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Mol	Chain	Res	Type
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	36	HIS
1	B	80	ASN
1	B	141	GLN
1	B	153	GLN
1	B	170	ASN
1	B	179	ASN
1	B	263	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	B	731	GLN
1	C	66	HIS
1	C	112	GLN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	344	GLN
1	C	369	ASN
1	C	455	GLN
1	C	572	ASN
1	C	586	GLN
1	C	685	ASN
1	C	697	GLN
1	C	710	ASN
1	D	75	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	272	ASN
1	D	344	GLN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS

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Mol	Chain	Res	Type
1	D	685	ASN
1	D	710	ASN
1	D	731	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 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	RUF	A	800	-	22,30,30	0.76	0	28,44,44	1.33	4 (14%)
3	NAG	A	801	1	14,14,15	0.62	0	17,19,21	1.25	1 (5%)
3	NAG	A	802	1	14,14,15	0.61	0	17,19,21	1.30	2 (11%)
3	NAG	A	803	1	14,14,15	0.78	0	17,19,21	1.25	1 (5%)
3	NAG	A	804	1,3	14,14,15	0.53	0	17,19,21	1.14	3 (17%)
3	NAG	A	805	3	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
3	NAG	A	806	1,3	14,14,15	0.57	0	17,19,21	1.82	5 (29%)
3	NAG	A	807	3	14,14,15	0.58	0	17,19,21	0.92	0
3	NAG	A	808	1	14,14,15	0.64	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RUF	B	800	-	22,30,30	0.77	0	28,44,44	1.51	4 (14%)
3	NAG	B	801	1	14,14,15	0.85	1 (7%)	17,19,21	1.63	5 (29%)
3	NAG	B	802	1	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
3	NAG	B	803	1	14,14,15	0.56	0	17,19,21	1.46	3 (17%)
3	NAG	B	804	1,3	14,14,15	0.68	0	17,19,21	1.16	3 (17%)
3	NAG	B	805	3	14,14,15	0.43	0	17,19,21	1.64	1 (5%)
3	NAG	B	806	1	14,14,15	0.54	0	17,19,21	1.21	2 (11%)
2	RUF	C	800	-	22,30,30	0.86	0	28,44,44	1.41	4 (14%)
3	NAG	C	801	1	14,14,15	0.54	0	17,19,21	1.36	1 (5%)
3	NAG	C	802	1	14,14,15	0.72	0	17,19,21	1.45	3 (17%)
3	NAG	C	803	1,3	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
3	NAG	C	804	3	14,14,15	0.50	0	17,19,21	0.75	0
2	RUF	D	800	-	22,30,30	0.67	0	28,44,44	1.32	4 (14%)
3	NAG	D	801	1	14,14,15	0.57	0	17,19,21	1.22	1 (5%)
3	NAG	D	802	1,3	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
3	NAG	D	803	3	14,14,15	0.55	0	17,19,21	1.21	1 (5%)
3	NAG	D	804	1	14,14,15	0.71	0	17,19,21	1.62	2 (11%)

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	RUF	A	800	-	-	0/4/16/16	0/4/4/4
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	807	3	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	RUF	B	800	-	-	0/4/16/16	0/4/4/4
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	805	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
2	RUF	C	800	-	-	0/4/16/16	0/4/4/4
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	804	3	-	0/6/23/26	0/1/1/1
2	RUF	D	800	-	-	0/4/16/16	0/4/4/4
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	3	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	NAG	C1-C2	2.40	1.55	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	RUF	C14-C13-N12	-5.17	104.74	113.31
2	C	800	RUF	C7-N6-C5	-4.09	112.88	121.81
2	A	800	RUF	C14-C13-N12	-3.99	106.69	113.31
3	D	802	NAG	O5-C1-C2	-3.80	106.28	111.52
2	B	800	RUF	C7-N6-C5	-3.60	113.96	121.81
2	D	800	RUF	C7-N6-C5	-3.37	114.45	121.81
2	A	800	RUF	C7-N6-C5	-3.30	114.62	121.81
2	D	800	RUF	C14-C13-N12	-3.13	108.11	113.31
3	A	804	NAG	O5-C1-C2	-2.99	107.39	111.52
2	C	800	RUF	C14-C13-N12	-2.95	108.42	113.31
2	D	800	RUF	C11-N6-C5	-2.66	116.00	121.81
3	A	806	NAG	O5-C1-C2	-2.59	107.95	111.52
3	A	806	NAG	C2-N2-C7	-2.56	119.20	122.94
2	B	800	RUF	C11-N6-C5	-2.55	116.25	121.81
2	C	800	RUF	C11-N6-C5	-2.49	116.38	121.81
3	B	804	NAG	C2-N2-C7	-2.48	119.32	122.94
3	A	806	NAG	C4-C3-C2	-2.32	107.62	111.02
3	A	808	NAG	O5-C1-C2	-2.30	108.34	111.52
3	B	801	NAG	O7-C7-C8	-2.19	118.11	122.07
3	C	803	NAG	O5-C1-C2	-2.17	108.53	111.52
3	B	803	NAG	O5-C1-C2	-2.09	108.64	111.52
2	A	800	RUF	C11-N6-C5	-2.03	117.38	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	NAG	O5-C1-C2	-2.01	108.74	111.52
3	B	803	NAG	C3-C4-C5	-2.00	106.66	110.24
3	A	804	NAG	O5-C5-C6	2.05	110.39	107.15
2	B	800	RUF	C13-N12-C5	2.05	128.37	124.87
3	C	802	NAG	C2-N2-C7	2.06	125.94	122.94
3	A	804	NAG	C4-C3-C2	2.08	114.06	111.02
3	B	804	NAG	O5-C5-C6	2.08	110.44	107.15
3	B	806	NAG	O5-C5-C6	2.17	110.58	107.15
2	D	800	RUF	C13-N12-C5	2.26	128.72	124.87
2	A	800	RUF	C13-N12-C5	2.46	129.07	124.87
2	C	800	RUF	C13-N12-C5	2.48	129.09	124.87
3	A	802	NAG	O5-C5-C6	2.49	111.08	107.15
3	C	802	NAG	O5-C5-C6	2.55	111.19	107.15
3	B	801	NAG	C2-N2-C7	2.59	126.72	122.94
3	D	803	NAG	C1-O5-C5	2.60	115.77	112.19
3	B	804	NAG	C4-C3-C2	2.74	115.03	111.02
3	B	802	NAG	C1-O5-C5	2.75	115.97	112.19
3	B	801	NAG	O5-C5-C6	2.75	111.50	107.15
3	A	806	NAG	C1-C2-N2	3.01	115.63	110.49
3	B	801	NAG	C4-C3-C2	3.08	115.53	111.02
3	B	801	NAG	C1-O5-C5	3.08	116.42	112.19
3	C	803	NAG	C4-C3-C2	3.21	115.72	111.02
3	B	806	NAG	C1-O5-C5	3.28	116.70	112.19
3	A	802	NAG	C1-O5-C5	3.35	116.80	112.19
3	D	804	NAG	C2-N2-C7	3.49	128.04	122.94
3	C	802	NAG	C4-C3-C2	3.54	116.20	111.02
3	A	803	NAG	C4-C3-C2	3.66	116.38	111.02
3	D	801	NAG	C1-O5-C5	3.78	117.39	112.19
3	C	801	NAG	C1-O5-C5	3.82	117.44	112.19
3	B	803	NAG	C1-O5-C5	3.89	117.54	112.19
3	A	801	NAG	C1-O5-C5	4.01	117.70	112.19
3	D	804	NAG	C1-O5-C5	4.19	117.95	112.19
3	A	806	NAG	C1-O5-C5	4.38	118.22	112.19
3	B	805	NAG	C1-O5-C5	5.65	119.96	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	RUF	2	0
2	B	800	RUF	2	0
2	C	800	RUF	4	0
2	D	800	RUF	2	0
3	D	801	NAG	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	723/740 (97%)	0.17	16 (2%) 62 62	35, 46, 62, 81	1 (0%)
1	B	729/740 (98%)	0.02	2 (0%) 93 94	37, 46, 63, 85	0
1	C	724/740 (97%)	0.29	39 (5%) 26 24	37, 46, 64, 82	0
1	D	724/740 (97%)	0.56	74 (10%) 7 5	35, 47, 63, 92	0
All	All	2900/2960 (97%)	0.26	131 (4%) 33 31	35, 46, 63, 92	1 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	GLU	7.6
1	D	88	VAL	5.7
1	D	467	TYR	5.3
1	D	415	LEU	4.8
1	C	88	VAL	4.6
1	C	89	PHE	4.6
1	D	99	GLY	4.5
1	D	416	TYR	4.5
1	D	333	SER	4.5
1	A	138	ASN	4.4
1	C	486	VAL	4.3
1	D	397	ILE	4.3
1	D	338	ASN	4.1
1	C	78	VAL	4.1
1	D	483	HIS	4.1
1	C	81	ALA	4.0
1	D	137	LEU	3.9
1	C	90	LEU	3.8
1	D	392	LYS	3.8
1	D	83	TYR	3.7
1	D	140	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	330	TYR	3.5
1	D	89	PHE	3.5
1	D	468	TYR	3.5
1	C	79	PHE	3.5
1	D	78	VAL	3.4
1	D	322	TYR	3.4
1	D	63	ILE	3.3
1	C	93	SER	3.3
1	D	273	THR	3.3
1	A	97	GLU	3.3
1	C	91	GLU	3.3
1	D	148	ILE	3.3
1	D	332	GLU	3.3
1	D	178	PRO	3.2
1	B	766	PRO	3.2
1	A	99	GLY	3.2
1	C	97	GLU	3.2
1	C	63	ILE	3.1
1	D	87	SER	3.0
1	C	330	TYR	3.0
1	D	77	LEU	3.0
1	A	93	SER	3.0
1	D	439	TYR	3.0
1	C	138	ASN	3.0
1	D	395	THR	3.0
1	C	335	GLY	3.0
1	D	396	PHE	2.9
1	C	83	TYR	2.9
1	D	372	TYR	2.9
1	D	92	ASN	2.9
1	D	464	GLU	2.9
1	A	86	SER	2.8
1	A	92	ASN	2.8
1	D	174	VAL	2.8
1	A	274	ASP	2.8
1	D	86	SER	2.8
1	D	62	TRP	2.8
1	D	331	ASP	2.8
1	D	348	MET	2.8
1	C	102	ILE	2.8
1	A	332	GLU	2.7
1	D	335	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	94	THR	2.7
1	C	95	PHE	2.7
1	C	76	ILE	2.7
1	C	96	ASP	2.7
1	D	100	HIS	2.6
1	C	179	ASN	2.6
1	D	135	TYR	2.6
1	A	489	LYS	2.6
1	A	96	ASP	2.6
1	D	339	CYS	2.6
1	D	393	ASP	2.6
1	D	346	ILE	2.6
1	C	100	HIS	2.6
1	A	279	VAL	2.6
1	A	333	SER	2.6
1	D	141	GLN	2.5
1	C	279	VAL	2.5
1	A	90	LEU	2.5
1	D	436	LEU	2.5
1	D	139	LYS	2.5
1	D	222	PHE	2.5
1	C	72	GLN	2.4
1	C	490	GLY	2.4
1	A	135	TYR	2.4
1	D	326	ASP	2.4
1	D	93	SER	2.4
1	D	414	TYR	2.4
1	C	87	SER	2.4
1	D	388	GLN	2.4
1	D	324	VAL	2.4
1	D	105	TYR	2.4
1	D	489	LYS	2.4
1	D	90	LEU	2.4
1	D	413	ASP	2.4
1	C	77	LEU	2.4
1	D	412	SER	2.4
1	D	279	VAL	2.3
1	D	347	GLU	2.3
1	C	489	LYS	2.3
1	D	487	ASN	2.3
1	D	274	ASP	2.3
1	C	333	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	141	GLN	2.2
1	D	173	TYR	2.2
1	D	386	TYR	2.2
1	D	138	ASN	2.2
1	D	384	ILE	2.2
1	C	334	SER	2.1
1	C	140	ARG	2.1
1	D	276	LEU	2.1
1	C	336	ARG	2.1
1	C	67	GLU	2.1
1	A	88	VAL	2.1
1	D	463	LYS	2.1
1	C	92	ASN	2.1
1	B	98	PHE	2.1
1	C	283	THR	2.1
1	D	385	CYS	2.1
1	D	394	CYS	2.1
1	C	86	SER	2.1
1	C	282	ALA	2.0
1	D	328	CYS	2.0
1	D	433	LYS	2.0
1	D	521	GLU	2.0
1	D	391	LYS	2.0
1	A	98	PHE	2.0
1	D	336	ARG	2.0
1	C	766	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. 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(\AA^2)	Q<0.9
3	NAG	A	803	14/15	0.71	0.28	61,64,69,69	0
3	NAG	B	801	14/15	0.72	0.17	68,70,71,71	0
3	NAG	D	801	14/15	0.73	0.21	55,57,57,58	0
3	NAG	B	805	14/15	0.75	0.26	74,76,78,79	0
3	NAG	C	801	14/15	0.78	0.25	52,53,55,56	0
3	NAG	A	801	14/15	0.79	0.19	58,60,61,61	0
3	NAG	C	804	14/15	0.79	0.23	74,76,78,79	0
3	NAG	A	806	14/15	0.80	0.16	63,67,69,71	0
3	NAG	D	803	14/15	0.81	0.21	61,64,66,67	0
3	NAG	D	804	14/15	0.81	0.16	73,76,78,78	0
3	NAG	B	803	14/15	0.82	0.21	58,61,64,64	0
3	NAG	C	802	14/15	0.83	0.23	58,61,64,64	0
3	NAG	B	802	14/15	0.83	0.21	56,60,62,64	0
3	NAG	B	806	14/15	0.84	0.12	61,63,66,66	0
3	NAG	A	807	14/15	0.84	0.15	74,75,76,77	0
3	NAG	A	805	14/15	0.88	0.15	61,62,64,65	0
3	NAG	A	802	14/15	0.89	0.23	65,68,68,69	0
3	NAG	A	808	14/15	0.90	0.20	54,58,60,60	0
3	NAG	B	804	14/15	0.92	0.16	55,61,65,70	0
3	NAG	C	803	14/15	0.94	0.14	60,63,67,71	0
2	RUF	D	800	27/27	0.94	0.25	51,53,54,55	0
3	NAG	D	802	14/15	0.94	0.12	51,53,55,58	0
3	NAG	A	804	14/15	0.94	0.14	52,54,57,59	0
2	RUF	A	800	27/27	0.95	0.26	52,55,58,59	0
2	RUF	B	800	27/27	0.96	0.28	54,55,59,59	0
2	RUF	C	800	27/27	0.97	0.24	53,55,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.