Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:49 AM GMT

PDB ID	:	2BUC
Title	:	CRYSTAL STRUCTURE OF PORCINE DIPEPTIDYL PEPTIDASE IV (CD26) IN COMPLEX WITH A TETRAHYDROISOQUINOLINE INHIBITOR
Authors	:	Nordhoff, S.; Cerezo-Galvez, S.; Feurer, A.; Hill, O.; Matassa, V.G.; Metz, G.; Rummey, C.; Thiemann, M.; Edwards, P.J.
Deposited on	:	2005-06-09
Resolution	:	2.50 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 (i)) were used in the production of this report:

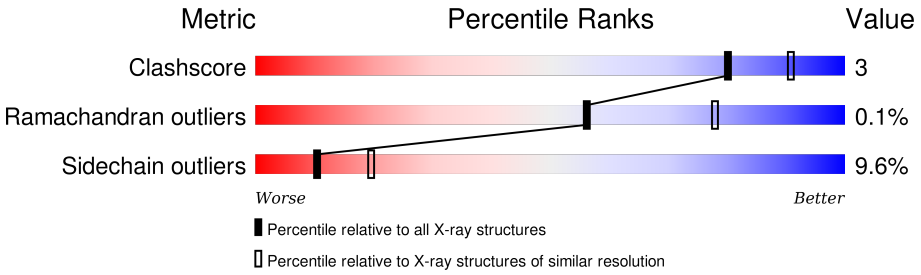
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	82% 16%
1	B	728	82% 16%
1	C	728	82% 16%
1	D	728	81% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1092	X	-	-	-
3	NAG	D	1092	X	-	-	-
4	NDG	D	1230	X	-	-	-
7	NDG	C	1092	X	-	-	-
7	NDG	D	1279	X	-	-	-

2 Entry composition

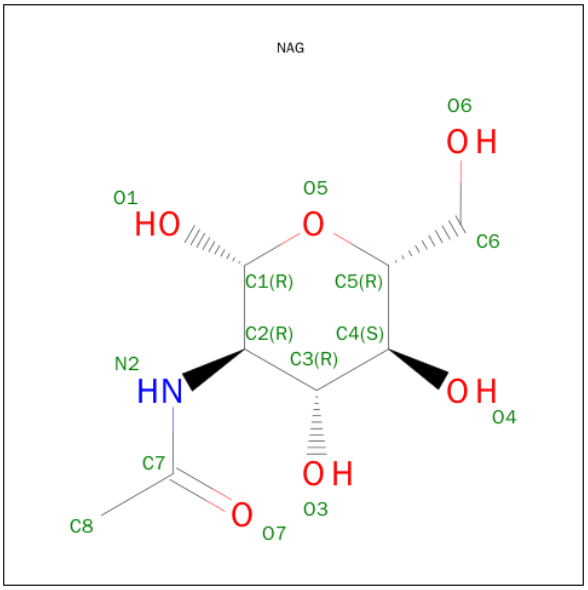
There are 9 unique types of molecules in this entry. The entry contains 25421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	0	0	0
			5966	3825	986	1132	23			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

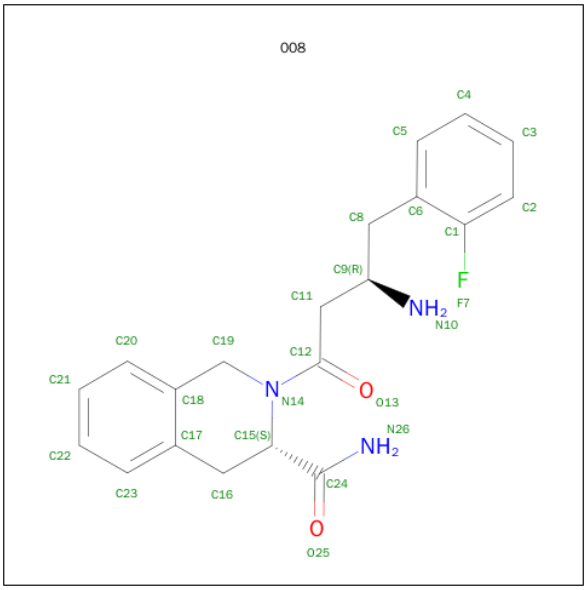
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total C N O 28 16 2 10	0	0
3	B	2	Total C N O 28 16 2 10	0	0
3	B	2	Total C N O 28 16 2 10	0	0
3	D	2	Total C N O 28 16 2 10	0	0
3	D	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

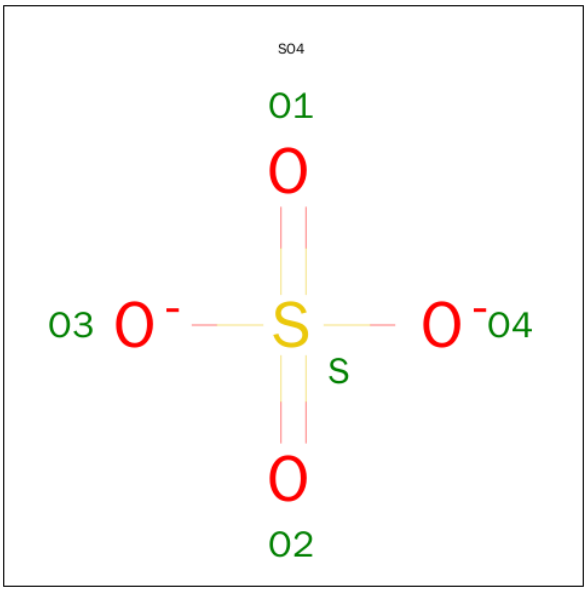
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total C N O 28 16 2 10	0	0
4	D	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is (S)-2-[(R)-3-AMINO-4-(2-FLUORO-PHENYL)-BUTYRYL]-1,2,3,4-TETRAHYDRO-ISOQUINOLINE-3-CARBOXYLIC ACID AMIDE (three-letter code: 008) (formula: $C_{20}H_{22}FN_3O_2$).



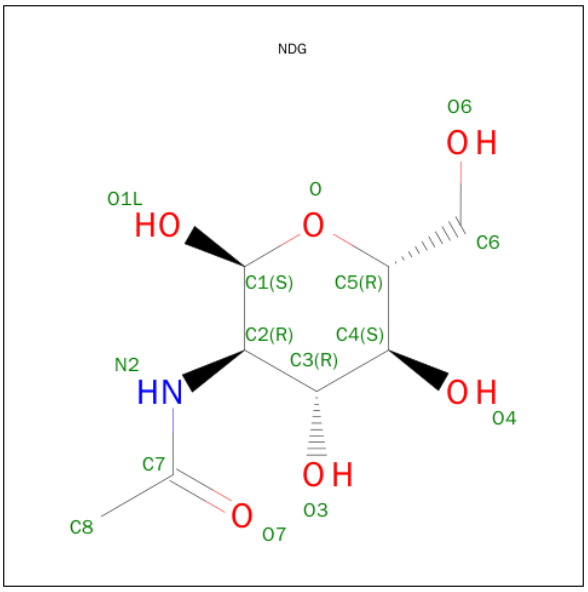
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
5	B	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
5	C	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
5	D	1	Total	C	F	N	O	0	0
			26	20	1	3	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total C N O 28 16 2 10	0	0
8	D	2	Total C N O 28 16 2 10	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	242	Total O 242 242	0	0
9	B	248	Total O 248 248	0	0
9	C	228	Total O 228 228	0	0
9	D	233	Total O 233 233	0	0

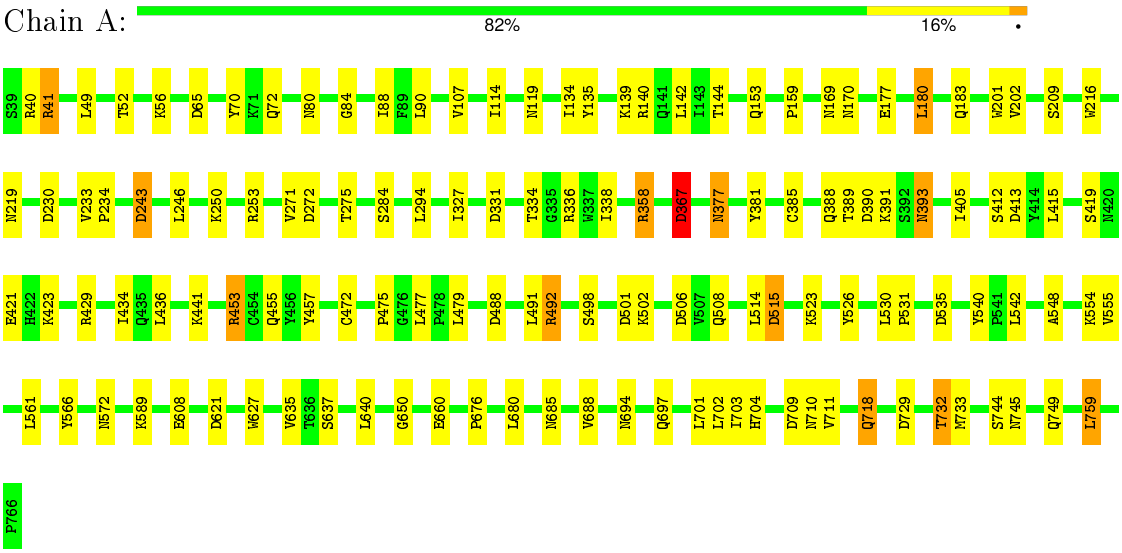
3 Residue-property plots (i)

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.

Note EDS was not executed.

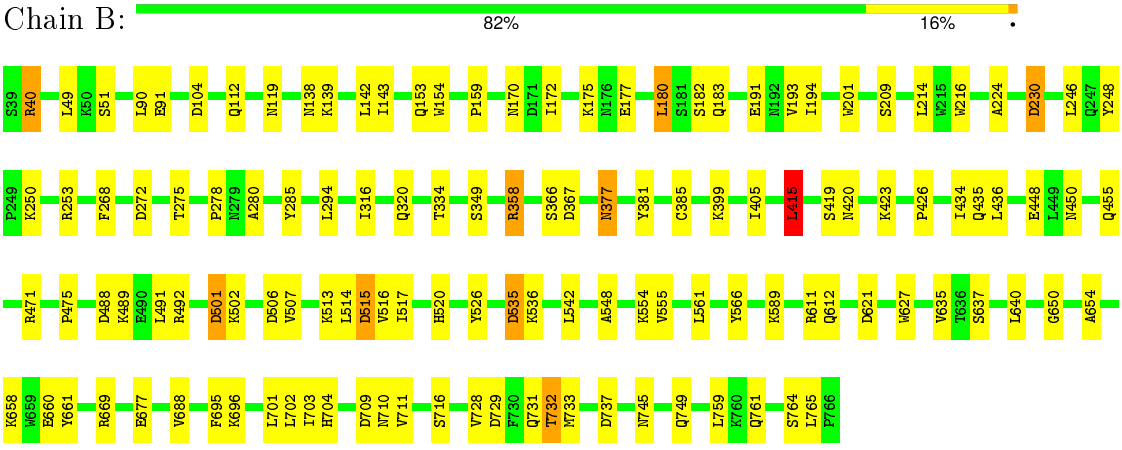
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain A:



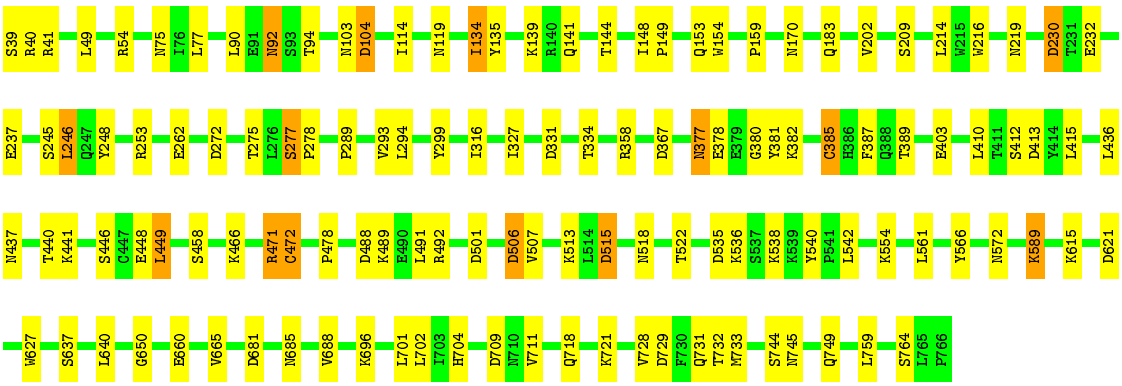
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain B:



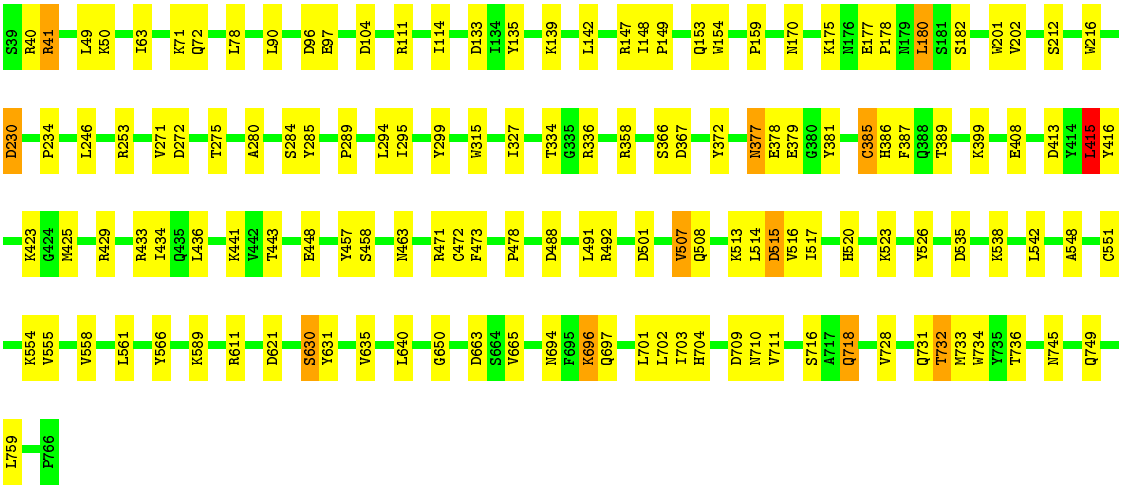
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain C:



- Molecule 1: DIPEPTIDYL PEPTIDASE IV

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.64Å 117.49Å 133.06Å 112.44° 94.72° 91.30°	Depositor
Resolution (Å)	19.28 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (19.28-2.50)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25421	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 008, NAG, NDG, SO4

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	0.31	0/6141	0.65	14/8353 (0.2%)
1	B	0.31	0/6141	0.65	14/8353 (0.2%)
1	C	0.32	0/6141	0.64	15/8353 (0.2%)
1	D	0.31	0/6141	0.64	14/8353 (0.2%)
All	All	0.31	0/24564	0.65	57/33412 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	1	0
4	D	1	0
All	All	2	0

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	272	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	390	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	535	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	535	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	272	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	535	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	515	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	243	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	415	LEU	CA-CB-CG	5.78	128.59	115.30
1	D	272	ASP	CB-CG-OD2	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	506	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	729	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	96	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	515	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	488	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	535	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	104	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	729	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	413	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	488	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	367	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	272	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	621	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	515	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	488	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	367	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	501	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	501	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	621	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	230	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	501	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	709	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	737	ASP	CB-CG-OD2	5.28	123.06	118.30
1	D	621	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	621	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	104	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	729	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	709	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	506	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	331	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	506	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	415	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	515	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	709	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	367	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	413	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	230	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	709	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	367	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	488	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	501	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	65	ASP	CB-CG-OD2	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	104	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	681	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	413	ASP	CB-CG-OD2	5.00	122.80	118.30
1	D	663	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1092	NAG	C1
4	D	1230	NDG	C1

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	5966	0	5661	47	0
1	B	5966	0	5662	44	0
1	C	5966	0	5662	41	0
1	D	5966	0	5660	48	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	0	0
3	A	28	0	25	0	0
3	B	56	0	50	0	0
3	D	56	0	50	0	0
4	A	28	0	25	0	0
4	D	28	0	25	0	0
5	A	26	0	22	1	0
5	B	26	0	22	1	0
5	C	26	0	22	0	0
5	D	26	0	22	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	10	0	0	0	0
7	C	14	0	13	0	0
7	D	28	0	26	0	0
8	C	28	0	25	0	0
8	D	28	0	25	0	0
9	A	242	0	0	1	0
9	B	248	0	0	1	0
9	C	228	0	0	0	0
9	D	233	0	0	1	0
All	All	25421	0	23153	162	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 (162) 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:D:551:CYS:SG	9:D:2188:HOH:O	2.41	0.78
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.37	0.73
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.71	0.70
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.75	0.68
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.42	0.67
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.91	0.66
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.61	0.65
1:A:453:ARG:HH21	1:A:477:LEU:HB2	1.62	0.64
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.80	0.63
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.81	0.62
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.61
1:B:377:ASN:ND2	1:B:381:TYR:H	2.01	0.58
1:B:285:TYR:HD1	1:D:280:ALA:HB2	1.67	0.58
1:C:377:ASN:ND2	1:C:381:TYR:H	2.03	0.57
1:A:331:ASP:HB2	1:A:338:ILE:HD11	1.86	0.57
1:B:358:ARG:HG2	5:B:1767:008:H22	1.86	0.57
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.86	0.57
1:A:377:ASN:ND2	1:A:381:TYR:H	2.03	0.56
1:B:377:ASN:HD22	1:B:377:ASN:C	2.07	0.56
1:A:733:MET:HA	1:B:732:THR:HG22	1.87	0.56
1:A:275:THR:HA	1:C:334:THR:O	2.06	0.56
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.88	0.55
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.89	0.55
1:B:637:SER:HB3	1:B:688:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.06	0.54
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.89	0.54
1:C:327:ILE:HD13	1:C:389:THR:HG23	1.90	0.54
1:B:704:HIS:HD2	1:B:716:SER:OG	1.90	0.54
1:D:694:ASN:HD22	1:D:697:GLN:HE22	1.54	0.53
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.90	0.53
1:A:540:TYR:HE2	1:A:572:ASN:HD22	1.55	0.53
1:A:429:ARG:HB2	1:A:457:TYR:H	1.74	0.53
1:D:377:ASN:HD22	1:D:377:ASN:C	2.12	0.52
1:C:446:SER:HA	1:C:449:LEU:HD12	1.92	0.52
1:A:107:VAL:HG22	1:A:114:ILE:HD12	1.92	0.52
1:A:201:TRP:CZ2	1:A:710:ASN:HA	2.45	0.52
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.91	0.52
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.92	0.52
1:A:526:TYR:HA	1:A:555:VAL:HG21	1.93	0.51
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.76	0.51
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.93	0.51
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.09	0.51
1:B:695:PHE:HB3	1:B:728:VAL:HG11	1.93	0.51
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.93	0.51
1:D:696:LYS:HG2	1:D:728:VAL:HG22	1.93	0.51
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.93	0.50
1:A:336:ARG:HD3	1:C:277:SER:OG	2.11	0.50
1:B:696:LYS:HG2	1:B:728:VAL:HG22	1.93	0.50
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.92	0.50
1:C:377:ASN:HD21	1:C:381:TYR:H	1.59	0.50
1:B:193:VAL:HG12	1:B:194:ILE:HG12	1.94	0.50
1:B:415:LEU:HB3	1:B:434:ILE:HG23	1.94	0.49
1:D:429:ARG:HB2	1:D:457:TYR:H	1.78	0.49
1:D:703:ILE:HG12	1:D:733:MET:HB3	1.94	0.49
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.77	0.49
1:A:732:THR:HG22	1:B:733:MET:HA	1.95	0.49
1:D:416:TYR:CE2	1:D:433:ARG:HD3	2.48	0.49
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.48	0.49
1:D:41:ARG:HD3	1:D:507:VAL:HG23	1.95	0.48
1:A:271:VAL:HG22	1:A:284:SER:HB3	1.96	0.48
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.79	0.48
1:C:75:ASN:OD1	1:C:92:ASN:HB3	2.14	0.48
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.95	0.48
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.96	0.47
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:HG3	1:D:182:SER:HB3	1.95	0.47
1:A:377:ASN:C	1:A:377:ASN:HD22	2.18	0.47
1:D:704:HIS:HD2	1:D:716:SER:OG	1.97	0.47
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.49	0.47
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.97	0.46
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.97	0.46
1:A:393:ASN:HD22	1:A:393:ASN:H	1.61	0.46
1:A:334:THR:O	1:C:275:THR:HA	2.15	0.46
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.15	0.46
1:C:733:MET:HA	1:D:732:THR:HG22	1.98	0.46
1:C:232:GLU:HB3	1:C:262:GLU:HG2	1.97	0.46
1:C:380:GLY:HA3	1:C:589:LYS:HE2	1.96	0.46
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.51	0.46
1:C:382:LYS:H	1:C:403:GLU:HG2	1.81	0.46
1:C:134:ILE:HD11	1:C:148:ILE:HD12	1.97	0.46
1:B:704:HIS:CD2	1:B:716:SER:OG	2.69	0.46
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.51	0.46
1:B:704:HIS:HE1	1:B:711:VAL:O	1.98	0.45
1:C:183:GLN:HE22	1:C:278:PRO:HA	1.81	0.45
1:B:172:ILE:HG12	1:B:214:LEU:HD21	1.97	0.45
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.98	0.45
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.98	0.45
1:D:271:VAL:HG22	1:D:284:SER:HB3	1.97	0.45
1:C:377:ASN:HD22	1:C:377:ASN:C	2.20	0.45
1:A:759:LEU:HD23	1:A:759:LEU:HA	1.86	0.45
1:B:405:ILE:HG12	1:B:419:SER:HA	1.99	0.45
1:C:704:HIS:HE1	1:C:711:VAL:O	1.99	0.45
1:A:694:ASN:HD22	1:A:697:GLN:HE22	1.63	0.45
1:D:377:ASN:ND2	1:D:381:TYR:H	2.15	0.44
1:B:526:TYR:HA	1:B:555:VAL:HG21	1.99	0.44
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.98	0.44
1:D:154:TRP:CD2	1:D:212:SER:HB3	2.52	0.44
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.53	0.44
1:A:367:ASP:HB2	9:A:2125:HOH:O	2.16	0.44
1:D:148:ILE:HA	1:D:149:PRO:HD3	1.90	0.44
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.48	0.44
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.44
1:C:299:TYR:CZ	1:C:665:VAL:HG22	2.53	0.44
1:C:540:TYR:HE2	1:C:572:ASN:HD22	1.66	0.44
1:A:377:ASN:HD21	1:A:381:TYR:H	1.64	0.44
1:B:154:TRP:HD1	1:B:214:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.00	0.43
1:C:289:PRO:HG2	1:C:294:LEU:HG	2.00	0.43
1:B:112:GLN:HG2	1:B:138:ASN:HD21	1.83	0.43
1:C:472:CYS:O	1:C:478:PRO:HA	2.19	0.43
1:D:526:TYR:HA	1:D:555:VAL:HG21	2.00	0.43
1:A:732:THR:CG2	1:B:733:MET:HA	2.48	0.43
1:B:420:ASN:HB2	1:B:426:PRO:HA	2.00	0.43
1:A:405:ILE:HG12	1:A:419:SER:HA	1.99	0.43
1:B:177:GLU:HB2	1:B:180:LEU:HB2	2.01	0.43
1:A:733:MET:HA	1:B:732:THR:CG2	2.48	0.43
1:B:377:ASN:HD21	1:B:381:TYR:H	1.66	0.42
1:D:372:TYR:CZ	1:D:386:HIS:HD2	2.37	0.42
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.67	0.42
1:C:41:ARG:HB3	1:C:507:VAL:HG23	2.00	0.42
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.55	0.42
1:A:70:TYR:CE2	1:A:72:GLN:HB2	2.54	0.42
1:C:704:HIS:CE1	1:C:711:VAL:O	2.73	0.42
1:C:385:CYS:HB3	1:C:387:PHE:CE1	2.55	0.42
1:A:637:SER:HB3	1:A:688:VAL:HG11	2.02	0.42
1:A:177:GLU:HB2	1:A:180:LEU:HB2	2.01	0.42
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.54	0.42
1:A:358:ARG:HG2	5:A:1767:008:H22	2.01	0.42
1:A:41:ARG:HG3	1:A:41:ARG:H	1.57	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.54	0.42
1:D:415:LEU:HB3	1:D:434:ILE:HG23	2.01	0.42
1:A:84:GLY:HA2	1:A:492:ARG:HH12	1.84	0.42
1:C:148:ILE:HA	1:C:149:PRO:HD3	1.92	0.41
1:D:630:SER:HB2	1:D:631:TYR:H	1.64	0.41
1:B:275:THR:HA	1:D:334:THR:O	2.19	0.41
1:D:133:ASP:HB3	1:D:142:LEU:HD21	2.02	0.41
1:B:316:ILE:HG12	1:B:320:GLN:HA	2.01	0.41
1:B:492:ARG:HD2	9:B:2178:HOH:O	2.19	0.41
1:A:233:VAL:HA	1:A:234:PRO:HD3	1.94	0.41
1:C:246:LEU:HD13	1:C:248:TYR:O	2.20	0.41
1:D:473:PHE:HB3	1:D:558:VAL:HG13	2.03	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:A:388:GLN:HB3	1:A:391:LYS:HB2	2.02	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.21	0.41
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.41
1:C:154:TRP:HD1	1:C:214:LEU:HD12	1.86	0.41
1:B:201:TRP:CZ2	1:B:710:ASN:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:HIS:HE1	1:A:711:VAL:O	2.03	0.41
1:C:637:SER:HB3	1:C:688:VAL:HG11	2.02	0.41
1:A:49:LEU:HD22	1:A:749:GLN:HA	2.03	0.41
1:A:676:PRO:HD3	1:A:680:LEU:HD22	2.03	0.41
1:C:733:MET:HA	1:D:732:THR:CG2	2.51	0.41
1:C:721:LYS:HB2	1:D:736:THR:HB	2.03	0.41
1:D:385:CYS:HB3	1:D:387:PHE:CE1	2.56	0.41
1:B:548:ALA:HB3	1:B:635:VAL:HG21	2.03	0.41
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.94	0.40
1:D:177:GLU:HA	1:D:178:PRO:HD3	1.93	0.40
1:C:458:SER:HB3	1:C:471:ARG:HB2	2.02	0.40
1:C:589:LYS:HD3	1:C:589:LYS:N	2.36	0.40
1:D:327:ILE:HD13	1:D:389:THR:HG23	2.02	0.40
1:B:153:GLN:HE22	1:B:170:ASN:ND2	2.19	0.40
1:B:334:THR:O	1:D:275:THR:HA	2.22	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	726/728 (100%)	693 (96%)	32 (4%)	1 (0%)	56	78
1	B	726/728 (100%)	697 (96%)	28 (4%)	1 (0%)	56	78
1	C	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	56	78
1	D	726/728 (100%)	696 (96%)	29 (4%)	1 (0%)	56	78
All	All	2904/2912 (100%)	2782 (96%)	118 (4%)	4 (0%)	56	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	40	ARG
1	D	40	ARG
1	C	40	ARG

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	652/652 (100%)	592 (91%)	60 (9%)	11	21
1	B	652/652 (100%)	590 (90%)	62 (10%)	11	20
1	C	652/652 (100%)	588 (90%)	64 (10%)	10	19
1	D	652/652 (100%)	588 (90%)	64 (10%)	10	19
All	All	2608/2608 (100%)	2358 (90%)	250 (10%)	10	19

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	52	THR
1	A	56	LYS
1	A	80	ASN
1	A	88	ILE
1	A	90	LEU
1	A	119	ASN
1	A	134	ILE
1	A	139	LYS
1	A	140	ARG
1	A	142	LEU
1	A	144	THR
1	A	169	ASN
1	A	180	LEU
1	A	183	GLN
1	A	202	VAL
1	A	209	SER
1	A	219	ASN

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Mol	Chain	Res	Type
1	A	230	ASP
1	A	243	ASP
1	A	246	LEU
1	A	250	LYS
1	A	294	LEU
1	A	358	ARG
1	A	367	ASP
1	A	377	ASN
1	A	385	CYS
1	A	393	ASN
1	A	412	SER
1	A	421	GLU
1	A	423	LYS
1	A	436	LEU
1	A	441	LYS
1	A	453	ARG
1	A	472	CYS
1	A	479	LEU
1	A	491	LEU
1	A	492	ARG
1	A	498	SER
1	A	502	LYS
1	A	508	GLN
1	A	514	LEU
1	A	515	ASP
1	A	523	LYS
1	A	542	LEU
1	A	554	LYS
1	A	561	LEU
1	A	566	TYR
1	A	589	LYS
1	A	608	GLU
1	A	627	TRP
1	A	660	GLU
1	A	685	ASN
1	A	701	LEU
1	A	702	LEU
1	A	718	GLN
1	A	732	THR
1	A	744	SER
1	A	745	ASN
1	A	759	LEU

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	51	SER
1	B	90	LEU
1	B	91	GLU
1	B	119	ASN
1	B	139	LYS
1	B	142	LEU
1	B	143	ILE
1	B	175	LYS
1	B	180	LEU
1	B	182	SER
1	B	191	GLU
1	B	209	SER
1	B	230	ASP
1	B	246	LEU
1	B	250	LYS
1	B	294	LEU
1	B	349	SER
1	B	358	ARG
1	B	366	SER
1	B	377	ASN
1	B	385	CYS
1	B	399	LYS
1	B	415	LEU
1	B	423	LYS
1	B	435	GLN
1	B	436	LEU
1	B	448	GLU
1	B	450	ASN
1	B	471	ARG
1	B	489	LYS
1	B	491	LEU
1	B	501	ASP
1	B	502	LYS
1	B	507	VAL
1	B	513	LYS
1	B	514	LEU
1	B	515	ASP
1	B	516	VAL
1	B	517	ILE
1	B	520	HIS
1	B	535	ASP

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Mol	Chain	Res	Type
1	B	536	LYS
1	B	542	LEU
1	B	554	LYS
1	B	561	LEU
1	B	566	TYR
1	B	589	LYS
1	B	611	ARG
1	B	612	GLN
1	B	627	TRP
1	B	660	GLU
1	B	677	GLU
1	B	701	LEU
1	B	702	LEU
1	B	731	GLN
1	B	732	THR
1	B	745	ASN
1	B	759	LEU
1	B	761	GLN
1	B	764	SER
1	B	765	LEU
1	C	39	SER
1	C	54	ARG
1	C	77	LEU
1	C	90	LEU
1	C	92	ASN
1	C	94	THR
1	C	103	ASN
1	C	104	ASP
1	C	119	ASN
1	C	134	ILE
1	C	139	LYS
1	C	141	GLN
1	C	144	THR
1	C	202	VAL
1	C	209	SER
1	C	219	ASN
1	C	230	ASP
1	C	245	SER
1	C	246	LEU
1	C	277	SER
1	C	293	VAL
1	C	316	ILE

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Mol	Chain	Res	Type
1	C	358	ARG
1	C	377	ASN
1	C	378	GLU
1	C	385	CYS
1	C	412	SER
1	C	436	LEU
1	C	437	ASN
1	C	440	THR
1	C	441	LYS
1	C	448	GLU
1	C	449	LEU
1	C	466	LYS
1	C	471	ARG
1	C	472	CYS
1	C	489	LYS
1	C	491	LEU
1	C	492	ARG
1	C	506	ASP
1	C	513	LYS
1	C	515	ASP
1	C	518	ASN
1	C	522	THR
1	C	536	LYS
1	C	538	LYS
1	C	542	LEU
1	C	554	LYS
1	C	561	LEU
1	C	566	TYR
1	C	589	LYS
1	C	615	LYS
1	C	627	TRP
1	C	660	GLU
1	C	685	ASN
1	C	701	LEU
1	C	702	LEU
1	C	718	GLN
1	C	731	GLN
1	C	732	THR
1	C	744	SER
1	C	745	ASN
1	C	759	LEU
1	C	764	SER

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Mol	Chain	Res	Type
1	D	41	ARG
1	D	50	LYS
1	D	63	ILE
1	D	71	LYS
1	D	72	GLN
1	D	78	LEU
1	D	90	LEU
1	D	97	GLU
1	D	111	ARG
1	D	139	LYS
1	D	147	ARG
1	D	180	LEU
1	D	202	VAL
1	D	230	ASP
1	D	246	LEU
1	D	294	LEU
1	D	295	ILE
1	D	336	ARG
1	D	358	ARG
1	D	366	SER
1	D	377	ASN
1	D	378	GLU
1	D	379	GLU
1	D	385	CYS
1	D	399	LYS
1	D	408	GLU
1	D	415	LEU
1	D	423	LYS
1	D	425	MET
1	D	436	LEU
1	D	441	LYS
1	D	443	THR
1	D	448	GLU
1	D	458	SER
1	D	463	ASN
1	D	471	ARG
1	D	491	LEU
1	D	492	ARG
1	D	507	VAL
1	D	508	GLN
1	D	513	LYS
1	D	514	LEU

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Mol	Chain	Res	Type
1	D	515	ASP
1	D	516	VAL
1	D	517	ILE
1	D	520	HIS
1	D	523	LYS
1	D	538	LYS
1	D	542	LEU
1	D	554	LYS
1	D	561	LEU
1	D	566	TYR
1	D	589	LYS
1	D	611	ARG
1	D	630	SER
1	D	696	LYS
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	731	GLN
1	D	732	THR
1	D	734	TRP
1	D	745	ASN
1	D	759	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	192	ASN
1	A	369	ASN
1	A	377	ASN
1	A	393	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	B	75	ASN
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	183	GLN
1	B	192	ASN
1	B	247	GLN
1	B	377	ASN
1	B	393	ASN
1	B	435	GLN
1	B	483	HIS
1	B	679	ASN
1	B	704	HIS
1	B	718	GLN
1	C	169	ASN
1	C	170	ASN
1	C	183	GLN
1	C	192	ASN
1	C	219	ASN
1	C	247	GLN
1	C	377	ASN
1	C	430	ASN
1	C	463	ASN
1	C	483	HIS
1	C	572	ASN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	D	75	ASN
1	D	138	ASN
1	D	170	ASN
1	D	176	ASN
1	D	192	ASN
1	D	247	GLN
1	D	369	ASN
1	D	377	ASN
1	D	386	HIS
1	D	463	ASN
1	D	483	HIS
1	D	679	ASN
1	D	694	ASN
1	D	697	GLN
1	D	704	HIS
1	D	718	GLN

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Mol	Chain	Res	Type
1	D	754	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

18 carbohydrates 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	$\#\|Z\| > 2$
3	NAG	A	1229	1,3	14,14,15	0.49	0	15,19,21	0.87	1 (6%)
3	NAG	A	1230	3	14,14,15	0.54	0	15,19,21	0.95	1 (6%)
4	NDG	A	1685	1,4	14,14,15	0.54	0	15,19,21	1.65	2 (13%)
4	NDG	A	1686	4	14,14,15	0.60	0	15,19,21	1.15	1 (6%)
3	NAG	B	1092	1,3	14,14,15	0.58	0	15,19,21	0.84	1 (6%)
3	NAG	B	1093	3	14,14,15	0.51	0	15,19,21	0.82	1 (6%)
3	NAG	B	1685	1,3	14,14,15	0.46	0	15,19,21	0.81	0
3	NAG	B	1686	3	14,14,15	0.49	0	15,19,21	1.02	1 (6%)
8	NAG	C	1685	1,8	14,14,15	0.47	0	15,19,21	0.85	0
8	NDG	C	1686	8	14,14,15	0.47	0	15,19,21	1.23	1 (6%)
3	NAG	D	1092	1,3	14,14,15	0.49	0	15,19,21	0.93	1 (6%)
3	NAG	D	1093	3	14,14,15	0.47	0	15,19,21	1.16	2 (13%)
4	NDG	D	1229	1,4	14,14,15	0.35	0	15,19,21	1.51	1 (6%)
4	NDG	D	1230	4	14,14,15	0.52	0	15,19,21	0.84	1 (6%)
8	NAG	D	1321	1,8	14,14,15	0.50	0	15,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NDG	D	1322	8	14,14,15	0.63	0	15,19,21	1.37	2 (13%)
3	NAG	D	1685	1,3	14,14,15	0.49	0	15,19,21	0.75	0
3	NAG	D	1686	3	14,14,15	0.49	0	15,19,21	0.85	0

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
3	NAG	A	1229	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1230	3	-	0/6/23/26	0/1/1/1
4	NDG	A	1685	1,4	-	0/6/23/26	0/1/1/1
4	NDG	A	1686	4	-	0/6/23/26	0/1/1/1
3	NAG	B	1092	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1093	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1685	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1686	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1685	1,8	-	0/6/23/26	0/1/1/1
8	NDG	C	1686	8	-	0/6/23/26	0/1/1/1
3	NAG	D	1092	1,3	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	D	1093	3	-	0/6/23/26	0/1/1/1
4	NDG	D	1229	1,4	-	0/6/23/26	0/1/1/1
4	NDG	D	1230	4	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	D	1321	1,8	-	0/6/23/26	0/1/1/1
8	NDG	D	1322	8	-	0/6/23/26	0/1/1/1
3	NAG	D	1685	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1686	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1093	NAG	C1-O5-C5	2.01	114.79	112.25
8	D	1322	NDG	C4-C3-C2	2.05	114.42	111.23
4	D	1230	NDG	C4-C3-C2	2.08	114.46	111.23
3	A	1229	NAG	C1-O5-C5	2.20	115.04	112.25
3	B	1092	NAG	C1-O5-C5	2.21	115.05	112.25
3	D	1093	NAG	C1-O5-C5	2.24	115.10	112.25
3	A	1230	NAG	C4-C3-C2	2.50	115.11	111.23
3	B	1686	NAG	C1-O5-C5	2.65	115.61	112.25
3	D	1093	NAG	C2-N2-C7	2.82	126.66	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1092	NAG	C1-O5-C5	3.01	116.07	112.25
4	A	1685	NDG	C1-O-C5	3.37	116.52	112.25
4	A	1686	NDG	C1-O-C5	3.70	116.95	112.25
8	C	1686	NDG	C1-O-C5	3.93	117.24	112.25
4	A	1685	NDG	O4-C4-C3	4.13	119.63	110.34
8	D	1322	NDG	C1-O-C5	4.22	117.61	112.25
4	D	1229	NDG	C1-O-C5	5.46	119.18	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1092	NAG	C1
4	D	1230	NDG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1092	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

27 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	NAG	A	1085	1	14,14,15	0.51	0	15,19,21	0.65	0
2	NAG	A	1092	1	14,14,15	0.58	0	15,19,21	0.85	0
2	NAG	A	1279	1	14,14,15	0.50	0	15,19,21	0.74	0
2	NAG	A	1321	1	14,14,15	0.47	0	15,19,21	0.80	0
5	008	A	1767	-	28,28,28	0.60	0	32,39,39	1.24	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	A	1768	-	4,4,4	0.22	0	6,6,6	0.10	0
6	SO4	A	1769	-	4,4,4	0.23	0	6,6,6	0.13	0
2	NAG	B	1085	1	14,14,15	0.45	0	15,19,21	0.78	1 (6%)
2	NAG	B	1229	1	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
2	NAG	B	1279	1	14,14,15	0.49	0	15,19,21	0.71	0
2	NAG	B	1321	1	14,14,15	0.50	0	15,19,21	0.79	0
5	008	B	1767	-	28,28,28	0.59	0	32,39,39	1.22	1 (3%)
6	SO4	B	1768	-	4,4,4	0.21	0	6,6,6	0.11	0
6	SO4	B	1769	-	4,4,4	0.21	0	6,6,6	0.09	0
2	NAG	C	1085	1	14,14,15	0.49	0	15,19,21	0.75	0
7	NDG	C	1092	1	14,14,15	0.48	0	15,19,21	0.67	0
2	NAG	C	1229	1	14,14,15	0.46	0	15,19,21	1.15	1 (6%)
2	NAG	C	1279	1	14,14,15	0.42	0	15,19,21	1.09	2 (13%)
2	NAG	C	1321	1	14,14,15	0.49	0	15,19,21	0.66	0
5	008	C	1767	-	28,28,28	0.57	0	32,39,39	1.14	1 (3%)
6	SO4	C	1768	-	4,4,4	0.20	0	6,6,6	0.12	0
6	SO4	C	1769	-	4,4,4	0.21	0	6,6,6	0.06	0
7	NDG	D	1085	1	14,14,15	0.51	0	15,19,21	1.44	3 (20%)
7	NDG	D	1279	1	14,14,15	0.48	0	15,19,21	0.71	0
5	008	D	1767	-	28,28,28	0.60	0	32,39,39	1.22	2 (6%)
6	SO4	D	1768	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	D	1769	-	4,4,4	0.20	0	6,6,6	0.09	0

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	NAG	A	1085	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1092	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	1279	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
5	008	A	1767	-	-	0/15/28/28	0/3/3/3
6	SO4	A	1768	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1769	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1085	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1229	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1279	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1321	1	-	0/6/23/26	0/1/1/1
5	008	B	1767	-	-	0/15/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	B	1768	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1769	-	-	0/0/0/0	0/0/0/0
2	NAG	C	1085	1	-	0/6/23/26	0/1/1/1
7	NDG	C	1092	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1229	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1279	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1321	1	-	0/6/23/26	0/1/1/1
5	008	C	1767	-	-	0/15/28/28	0/3/3/3
6	SO4	C	1768	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1769	-	-	0/0/0/0	0/0/0/0
7	NDG	D	1085	1	-	0/6/23/26	0/1/1/1
7	NDG	D	1279	1	1/1/5/7	0/6/23/26	0/1/1/1
5	008	D	1767	-	-	0/15/28/28	0/3/3/3
6	SO4	D	1768	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1769	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1767	008	C19-C18-C17	-2.21	116.07	120.69
2	C	1279	NAG	C1-O5-C5	2.01	114.80	112.25
7	D	1085	NDG	C4-C3-C2	2.07	114.45	111.23
2	B	1229	NAG	C1-O5-C5	2.09	114.91	112.25
2	C	1279	NAG	C3-C4-C5	2.19	114.01	110.20
2	B	1085	NAG	C1-O5-C5	2.30	115.16	112.25
5	D	1767	008	C16-C15-N14	2.67	112.83	109.87
2	C	1229	NAG	C1-O5-C5	2.95	116.00	112.25
5	C	1767	008	C16-C15-N14	3.03	113.23	109.87
7	D	1085	NDG	C3-C4-C5	3.09	115.58	110.20
7	D	1085	NDG	C1-O-C5	3.33	116.48	112.25
5	B	1767	008	C16-C15-N14	3.40	113.65	109.87
5	A	1767	008	C16-C15-N14	3.90	114.21	109.87

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	1092	NDG	C1
2	A	1092	NAG	C1
7	D	1279	NDG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1092	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1767	008	1	0
5	B	1767	008	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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.