



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:56 am GMT

PDB ID : 3NOX
Title : Crystal structure of human DPP-IV in complex with Sa-(+)-(6-(aminomethyl)-5-(2,4-dichlorophenyl)-7-methylimidazo[1,2-a]pyrimidin-2-yl)(morpholino) methanone
Authors : Klei, H.E.
Deposited on : 2010-06-25
Resolution : 2.34 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

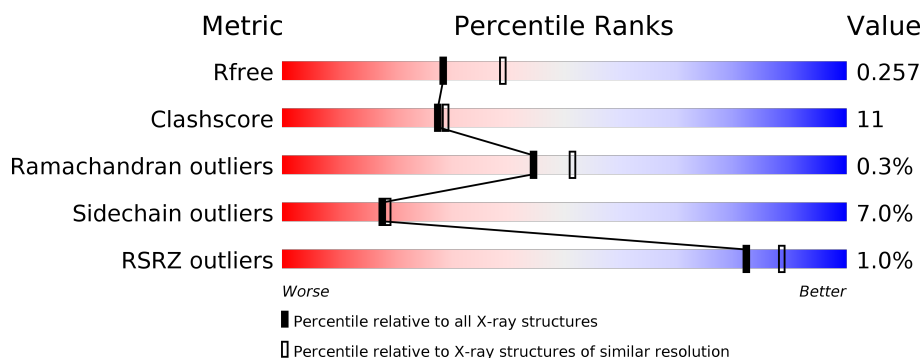
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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	753	
1	B	753	

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	2191	-	-	-	X
2	NAG	A	5201	-	-	-	X
2	NAG	B	1501	X	-	-	X
2	NAG	B	2191	-	-	-	X
2	NAG	B	5201	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12620 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 (CD26, adenosine deaminase complexing protein 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5940	3817	973	1124	26			
1	B	727	Total	C	N	O	S	0	1	0
			5943	3819	977	1121	26			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLU	-	EXPRESSION TAG	UNP Q53TN1
A	38	PHE	-	EXPRESSION TAG	UNP Q53TN1
A	767	PRO	-	EXPRESSION TAG	UNP Q53TN1
A	768	LEU	-	EXPRESSION TAG	UNP Q53TN1
A	769	GLU	-	EXPRESSION TAG	UNP Q53TN1
A	770	GLN	-	EXPRESSION TAG	UNP Q53TN1
A	771	LYS	-	EXPRESSION TAG	UNP Q53TN1
A	772	LEU	-	EXPRESSION TAG	UNP Q53TN1
A	773	ILE	-	EXPRESSION TAG	UNP Q53TN1
A	774	SER	-	EXPRESSION TAG	UNP Q53TN1
A	775	GLU	-	EXPRESSION TAG	UNP Q53TN1
A	776	GLU	-	EXPRESSION TAG	UNP Q53TN1
A	777	ASP	-	EXPRESSION TAG	UNP Q53TN1
A	778	LEU	-	EXPRESSION TAG	UNP Q53TN1
A	779	ASN	-	EXPRESSION TAG	UNP Q53TN1
A	780	SER	-	EXPRESSION TAG	UNP Q53TN1
A	781	ALA	-	EXPRESSION TAG	UNP Q53TN1
A	782	VAL	-	EXPRESSION TAG	UNP Q53TN1
A	783	ASP	-	EXPRESSION TAG	UNP Q53TN1
A	784	HIS	-	EXPRESSION TAG	UNP Q53TN1
A	785	HIS	-	EXPRESSION TAG	UNP Q53TN1
A	786	HIS	-	EXPRESSION TAG	UNP Q53TN1
A	787	HIS	-	EXPRESSION TAG	UNP Q53TN1
A	788	HIS	-	EXPRESSION TAG	UNP Q53TN1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	789	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	37	GLU	-	EXPRESSION TAG	UNP Q53TN1
B	38	PHE	-	EXPRESSION TAG	UNP Q53TN1
B	767	PRO	-	EXPRESSION TAG	UNP Q53TN1
B	768	LEU	-	EXPRESSION TAG	UNP Q53TN1
B	769	GLU	-	EXPRESSION TAG	UNP Q53TN1
B	770	GLN	-	EXPRESSION TAG	UNP Q53TN1
B	771	LYS	-	EXPRESSION TAG	UNP Q53TN1
B	772	LEU	-	EXPRESSION TAG	UNP Q53TN1
B	773	ILE	-	EXPRESSION TAG	UNP Q53TN1
B	774	SER	-	EXPRESSION TAG	UNP Q53TN1
B	775	GLU	-	EXPRESSION TAG	UNP Q53TN1
B	776	GLU	-	EXPRESSION TAG	UNP Q53TN1
B	777	ASP	-	EXPRESSION TAG	UNP Q53TN1
B	778	LEU	-	EXPRESSION TAG	UNP Q53TN1
B	779	ASN	-	EXPRESSION TAG	UNP Q53TN1
B	780	SER	-	EXPRESSION TAG	UNP Q53TN1
B	781	ALA	-	EXPRESSION TAG	UNP Q53TN1
B	782	VAL	-	EXPRESSION TAG	UNP Q53TN1
B	783	ASP	-	EXPRESSION TAG	UNP Q53TN1
B	784	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	785	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	786	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	787	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	788	HIS	-	EXPRESSION TAG	UNP Q53TN1
B	789	HIS	-	EXPRESSION TAG	UNP Q53TN1

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

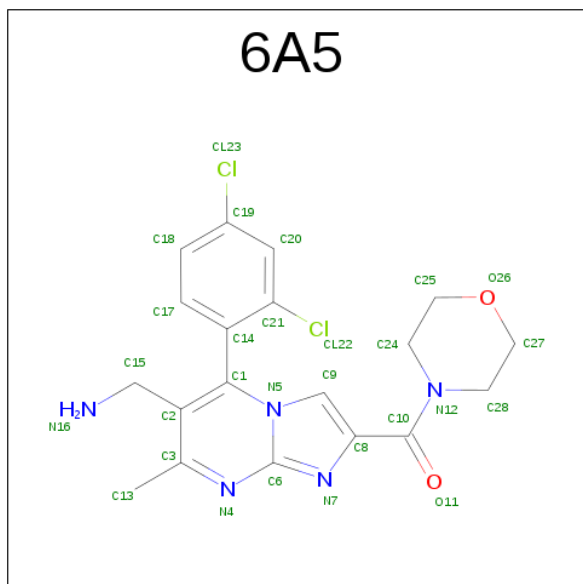


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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

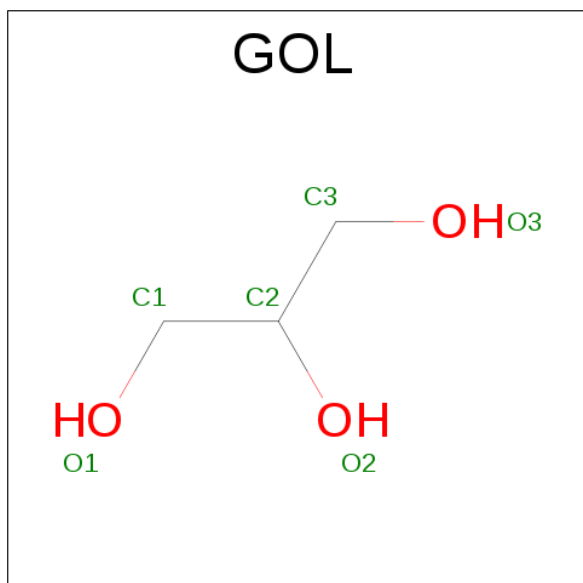
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SA-(+)-(6-(AMINOMETHYL)-5-(2,4-DICHLOROPHENYL)-7-METHYLMIDAZO[1,2-A]PYRIMIDIN-2-YL)(MORPHOLINO)METHANONE (three-letter code: 6A5) (formula: $C_{19}H_{19}Cl_2N_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			28	19	2	5	2		
4	B	1	Total	C	Cl	N	O	0	0
			28	19	2	5	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

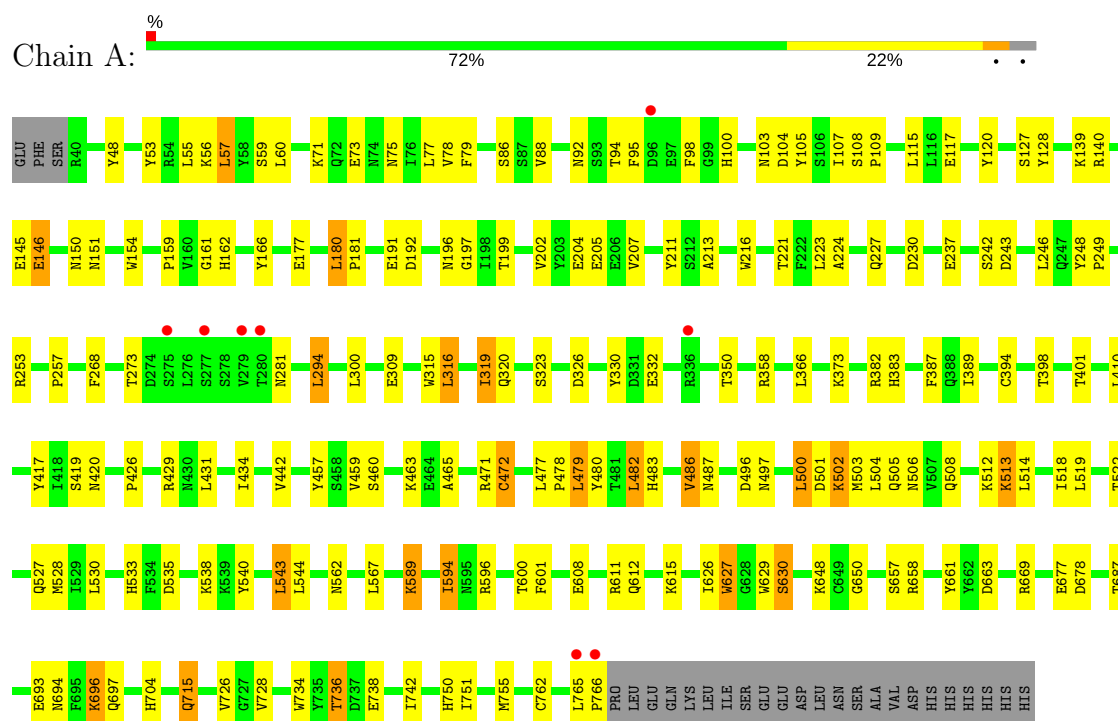
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total	O	0	0
			224	224		
6	B	255	Total	O	0	0
			255	255		

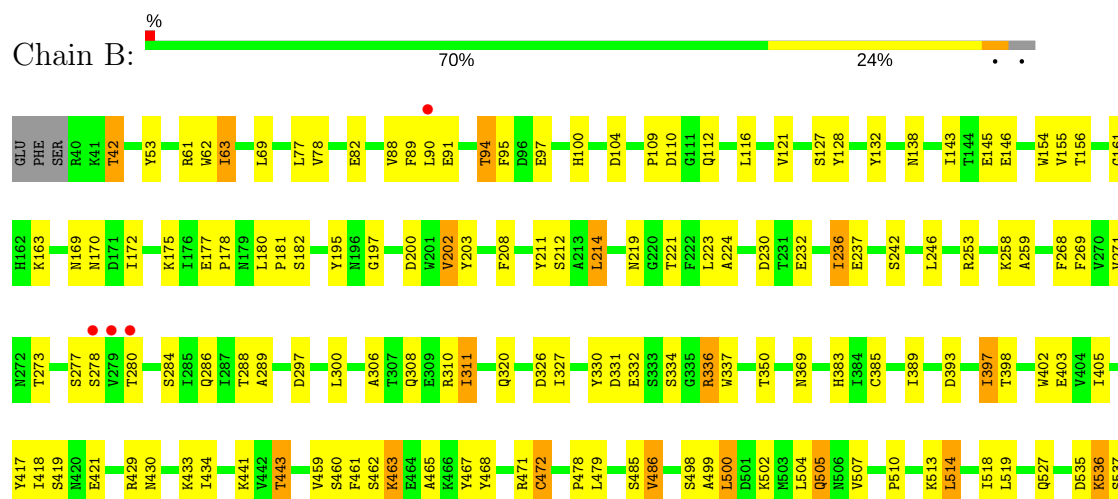
3 Residue-property plots

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 (CD26, adenosine deaminase complexing protein 2)



- Molecule 1: Dipeptidyl-peptidase 4 (CD26, adenosine deaminase complexing protein 2)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.45Å 67.07Å 420.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.62 – 2.34 35.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	86.1 (35.62-2.34) 86.1 (35.62-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.34Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_446)	Depositor
R, R_{free}	0.196 , 0.264 0.190 , 0.257	Depositor DCC
R_{free} test set	1539 reflections (2.24%)	DCC
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: GOL, NAG, 6A5

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	0.42	0/6112	0.57	0/8316
1	B	0.43	0/6118	0.60	0/8324
All	All	0.42	0/12230	0.58	0/16640

There are no bond length outliers.

There are no bond angle outliers.

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	5940	0	5633	134	0
1	B	5943	0	5639	136	0
2	A	70	0	65	4	0
2	B	70	0	65	1	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	28	0	19	1	0
4	B	28	0	19	0	0
5	B	6	0	8	1	0
6	A	224	0	0	6	0
6	B	255	0	0	5	0
All	All	12620	0	11498	266	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 11.

All (266) 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:273:THR:HB	6:A:805:HOH:O	1.49	1.12
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.40	1.03
1:B:600:THR:HG22	1:B:601:PHE:H	1.31	0.95
1:B:600:THR:HG22	1:B:601:PHE:N	1.83	0.93
1:A:319:ILE:HD12	1:A:319:ILE:H	1.34	0.92
1:B:236:ILE:HG13	1:B:712:HIS:CE1	2.07	0.90
1:A:281:ASN:HD21	2:A:2811:NAG:C1	1.87	0.87
1:B:91:GLU:CD	1:B:91:GLU:H	1.80	0.85
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.61	0.83
1:B:443:THR:HG22	6:B:875:HOH:O	1.80	0.82
1:A:693:GLU:O	1:A:696:LYS:HG3	1.82	0.80
1:A:253:ARG:NH1	1:B:253:ARG:HH12	1.80	0.79
1:A:736:THR:HG21	1:B:717:ALA:O	1.83	0.79
1:A:253:ARG:HH12	1:B:253:ARG:HH12	1.36	0.73
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.18	0.73
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.70	0.72
1:B:518:ILE:O	1:B:519:LEU:HD12	1.90	0.72
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.23	0.71
1:A:420:ASN:ND2	1:A:426:PRO:HA	2.04	0.71
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.71	0.71
1:B:397:ILE:HG23	1:B:434:ILE:HD13	1.73	0.71
1:B:600:THR:CG2	1:B:601:PHE:N	2.55	0.70
1:B:138:ASN:HB2	6:B:869:HOH:O	1.94	0.67
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.76	0.67
1:A:429:ARG:HD2	6:A:794:HOH:O	1.94	0.66
1:A:56:LYS:HE3	1:A:497:ASN:HA	1.77	0.66
1:A:471:ARG:HD2	1:A:480:TYR:HE1	1.61	0.66
1:A:103:ASN:HB3	1:A:117:GLU:O	1.96	0.65
1:B:221:THR:HG21	2:B:2191:NAG:H5	1.79	0.65
1:B:505:GLN:HE21	1:B:505:GLN:HA	1.61	0.65
1:A:543:LEU:HD21	1:A:627:TRP:HD1	1.62	0.65
1:A:71:LYS:HE2	1:A:105:TYR:OH	1.97	0.64
1:A:109:PRO:HD2	1:A:161:GLY:O	1.98	0.64
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.32	0.64
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.78	0.64
1:B:622:LYS:HB2	1:B:622:LYS:NZ	2.13	0.64
1:A:518:ILE:O	1:A:519:LEU:HD23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:NZ	1:A:697:GLN:HE21	1.95	0.63
1:B:405:ILE:HD12	1:B:419:SER:HA	1.80	0.63
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.81	0.62
1:B:597:ARG:O	1:B:600:THR:HB	2.00	0.62
1:A:281:ASN:HD21	2:A:2811:NAG:C2	2.13	0.61
1:A:281:ASN:ND2	2:A:2811:NAG:C1	2.62	0.61
1:A:420:ASN:HD22	1:A:426:PRO:HA	1.66	0.61
1:A:589:LYS:HE3	1:A:589:LYS:O	2.01	0.61
1:B:596:ARG:NH2	1:B:678:ASP:OD1	2.33	0.60
1:A:477:LEU:HD12	1:A:501:ASP:HB2	1.83	0.60
1:A:726:VAL:HG22	1:A:726:VAL:O	2.00	0.60
1:A:253:ARG:HH12	1:B:253:ARG:NH1	1.98	0.60
1:B:208:PHE:HZ	1:B:300:LEU:HD12	1.67	0.60
1:B:536:LYS:H	1:B:536:LYS:HD3	1.68	0.59
1:A:319:ILE:CD1	1:A:319:ILE:H	2.07	0.59
1:A:694:ASN:HA	1:A:696:LYS:NZ	2.18	0.59
1:B:402:TRP:CD1	1:B:421:GLU:HG3	2.37	0.59
1:A:608:GLU:OE1	1:A:608:GLU:HA	2.03	0.58
1:B:405:ILE:HD13	1:B:429:ARG:HD3	1.85	0.58
1:A:657:SER:H	1:A:715:GLN:NE2	2.02	0.58
1:B:42:THR:HG23	1:B:570:THR:OG1	2.04	0.58
1:A:205:GLU:OE2	4:A:1:6A5:N16	2.36	0.58
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.04	0.58
1:A:202:VAL:CG1	1:A:257:PRO:HD2	2.34	0.57
1:A:309:GLU:HG2	2:A:2191:NAG:H62	1.86	0.57
1:A:127:SER:HB3	1:A:211:TYR:CG	2.39	0.57
1:B:219:ASN:HB2	1:B:308:GLN:OE1	2.04	0.57
1:B:397:ILE:HG22	1:B:398:THR:HG23	1.87	0.56
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.41	0.56
1:B:330:TYR:CE2	1:B:332:GLU:HA	2.41	0.55
1:A:477:LEU:CD1	1:A:501:ASP:HB2	2.37	0.55
1:B:397:ILE:CG2	1:B:434:ILE:HD13	2.36	0.55
1:B:100:HIS:CD2	6:B:973:HOH:O	2.60	0.55
1:A:107:ILE:HG22	1:A:108:SER:O	2.07	0.55
1:B:177:GLU:CB	1:B:180:LEU:HD23	2.26	0.55
1:A:315:TRP:O	1:A:323:SER:HB2	2.06	0.54
1:B:562:ASN:HD22	1:B:562:ASN:C	2.08	0.54
1:B:77:LEU:HD23	1:B:88:VAL:HA	1.88	0.54
1:A:197:GLY:C	1:A:213:ALA:HB3	2.29	0.53
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.90	0.53
1:B:271:VAL:HG22	1:B:284:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.43	0.53
1:B:459:VAL:HG22	1:B:460:SER:N	2.23	0.53
1:B:271:VAL:CG2	1:B:284:SER:HB3	2.38	0.53
1:B:277:SER:HB3	1:B:280:THR:HB	1.91	0.53
1:A:202:VAL:HG11	1:A:257:PRO:HD2	1.91	0.52
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.92	0.52
1:B:91:GLU:CD	1:B:91:GLU:N	2.57	0.52
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.75	0.52
1:B:297:ASP:HB3	6:B:864:HOH:O	2.10	0.52
1:B:121:VAL:O	1:B:128:TYR:HB2	2.08	0.52
1:A:502:LYS:HG3	1:A:503:MET:N	2.25	0.52
1:A:696:LYS:HD2	1:A:697:GLN:HG3	1.91	0.52
1:A:696:LYS:HZ3	1:A:697:GLN:HE21	1.56	0.52
1:A:508:GLN:NE2	1:A:533:HIS:HE1	2.08	0.51
1:B:383:HIS:CD2	1:B:398:THR:OG1	2.63	0.51
1:A:479:LEU:HD23	1:A:496:ASP:HA	1.92	0.51
1:A:57:LEU:HA	1:A:480:TYR:CE2	2.45	0.51
1:A:146:GLU:HG3	1:A:181:PRO:N	2.26	0.51
1:A:75:ASN:HD21	1:A:92:ASN:ND2	2.08	0.51
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.41	0.51
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.46	0.51
1:B:383:HIS:HD2	1:B:398:THR:OG1	1.93	0.51
1:A:508:GLN:HE21	1:A:533:HIS:CE1	2.28	0.51
1:A:434:ILE:HG12	1:A:442:VAL:HG22	1.93	0.51
1:A:60:LEU:O	1:A:60:LEU:HD12	2.12	0.51
1:B:163:LYS:HD3	1:B:273:THR:HG21	1.92	0.50
1:A:486:VAL:HG23	1:A:487:ASN:H	1.76	0.50
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.47	0.50
1:A:401:THR:HG22	1:A:401:THR:O	2.12	0.50
1:A:417:TYR:HE1	1:A:434:ILE:HG13	1.76	0.50
1:A:611:ARG:O	1:A:615:LYS:HG3	2.12	0.50
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.11	0.50
1:A:503:MET:O	1:A:506:ASN:HB2	2.12	0.49
1:B:742:ILE:HG22	1:B:742:ILE:O	2.11	0.49
1:A:594:ILE:HD12	1:A:601:PHE:HB2	1.94	0.49
1:B:221:THR:O	1:B:273:THR:HB	2.13	0.49
1:A:501:ASP:O	1:A:505:GLN:HG3	2.13	0.49
1:A:71:LYS:HE3	6:A:815:HOH:O	2.12	0.49
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.94	0.49
1:B:626:ILE:O	1:B:650:GLY:HA2	2.13	0.48
1:B:535:ASP:OD1	1:B:537:SER:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:THR:OG1	1:A:601:PHE:N	2.44	0.48
1:A:612:GLN:NE2	1:A:615:LYS:HD2	2.28	0.48
1:A:657:SER:H	1:A:715:GLN:HE21	1.61	0.48
1:B:417:TYR:HE1	1:B:419:SER:HB3	1.78	0.48
1:B:94:THR:O	1:B:95:PHE:HB2	2.13	0.48
1:B:63:ILE:HD11	1:B:69:LEU:HD12	1.95	0.48
1:A:79:PHE:CD2	1:A:86:SER:HB3	2.48	0.48
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.96	0.48
1:A:648:LYS:HE2	1:A:762:CYS:O	2.14	0.48
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.94	0.48
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.82	0.48
1:A:145:GLU:O	1:A:146:GLU:C	2.52	0.47
1:B:172:ILE:HD11	1:B:197:GLY:HA3	1.96	0.47
1:B:53:TYR:HB3	1:B:500:LEU:HD21	1.95	0.47
1:A:482:LEU:C	1:A:483:HIS:CD2	2.88	0.47
1:A:48:TYR:CE1	1:A:562:ASN:HA	2.49	0.47
1:A:387:PHE:CE2	1:A:394:CYS:HB3	2.49	0.47
1:B:513:LYS:O	1:B:527:GLN:HA	2.14	0.47
1:A:750:HIS:CG	1:B:724:VAL:HG22	2.49	0.47
1:B:608:GLU:O	1:B:612:GLN:HG2	2.15	0.47
1:A:207:VAL:HA	1:A:358:ARG:HH12	1.79	0.47
1:B:219:ASN:HB3	1:B:221:THR:OG1	2.15	0.47
1:B:745:SER:O	1:B:749:GLN:HG3	2.14	0.47
1:B:463:LYS:C	1:B:465:ALA:H	2.17	0.47
1:A:191:GLU:HG2	1:A:192:ASP:OD2	2.14	0.47
1:B:127:SER:HB3	1:B:211:TYR:CG	2.50	0.47
1:B:288:THR:HG22	1:B:289:ALA:O	2.15	0.47
1:B:595:ASN:O	1:B:597:ARG:HD3	2.15	0.47
1:A:751:ILE:O	1:A:755:MET:HG3	2.15	0.46
1:A:95:PHE:HA	6:A:998:HOH:O	2.14	0.46
1:A:457:TYR:CE1	1:A:472:CYS:HB2	2.51	0.46
1:A:629:TRP:HD1	1:A:630:SER:N	2.14	0.46
1:B:236:ILE:HG13	1:B:712:HIS:ND1	2.30	0.46
1:B:180:LEU:N	1:B:180:LEU:HD22	2.31	0.46
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.97	0.46
1:B:258:LYS:O	1:B:259:ALA:C	2.54	0.46
1:B:405:ILE:HD12	1:B:419:SER:CA	2.44	0.46
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.98	0.46
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.97	0.46
1:A:60:LEU:C	1:A:60:LEU:HD12	2.37	0.45
1:B:42:THR:HG21	1:B:570:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASP:O	1:B:589:LYS:C	2.52	0.45
1:B:594:ILE:HD11	1:B:602:GLU:OE1	2.16	0.45
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.52	0.45
1:A:55:LEU:HD22	1:A:478:PRO:HG2	1.99	0.45
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.17	0.45
1:A:629:TRP:CD1	1:A:630:SER:N	2.85	0.45
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.31	0.45
1:A:738:GLU:OE1	1:A:742:ILE:HA	2.16	0.45
1:A:88:VAL:HG13	1:A:88:VAL:O	2.17	0.45
1:B:200:ASP:OD1	1:B:203:TYR:HB2	2.16	0.45
1:A:538:LYS:HB2	1:A:540:TYR:CE1	2.52	0.45
1:B:154:TRP:HD1	1:B:214:LEU:HD22	1.82	0.45
1:A:73:GLU:O	1:A:73:GLU:HG2	2.17	0.45
1:B:417:TYR:CE1	1:B:419:SER:HB3	2.52	0.45
1:B:614:SER:O	1:B:616:MET:O	2.34	0.45
1:B:693:GLU:O	1:B:696:LYS:HG3	2.17	0.45
1:A:94:THR:O	1:A:95:PHE:HB2	2.17	0.44
1:B:514:LEU:HD12	1:B:557:THR:HG22	2.00	0.44
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.52	0.44
1:A:221:THR:HA	6:A:805:HOH:O	2.17	0.44
1:A:330:TYR:HE2	1:A:332:GLU:HG2	1.83	0.44
1:A:508:GLN:HE21	1:A:533:HIS:HE1	1.65	0.44
1:B:418:ILE:HA	1:B:430:ASN:O	2.18	0.44
1:B:640:LEU:HD12	1:B:700:TYR:CD1	2.52	0.44
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.52	0.44
1:B:334:SER:OG	1:B:336:ARG:HG2	2.18	0.44
1:B:95:PHE:C	1:B:97:GLU:H	2.21	0.44
1:A:53:TYR:HB3	1:A:500:LEU:HD21	1.98	0.44
1:B:169:ASN:O	1:B:170:ASN:HB2	2.17	0.44
1:A:459:VAL:HG22	1:A:460:SER:N	2.33	0.44
1:B:726:VAL:HG13	1:B:726:VAL:O	2.18	0.44
1:B:600:THR:HG22	1:B:601:PHE:CG	2.53	0.43
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.00	0.43
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.81	0.43
1:A:694:ASN:HA	1:A:696:LYS:HZ3	1.81	0.43
1:B:110:ASP:CG	1:B:112:GLN:HG3	2.38	0.43
1:B:306:ALA:CB	1:B:310:ARG:HG2	2.41	0.43
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.17	0.43
1:A:535:ASP:HB3	1:A:538:LYS:HG3	2.01	0.43
1:B:675:THR:HB	1:B:677:GLU:OE1	2.17	0.43
1:A:463:LYS:C	1:A:465:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:H	1:A:60:LEU:HG	1.71	0.43
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.18	0.43
1:A:626:ILE:O	1:A:650:GLY:HA2	2.19	0.43
1:B:499:ALA:HA	1:B:502:LYS:HE2	2.00	0.43
1:B:622:LYS:HB2	1:B:622:LYS:HZ1	1.82	0.43
1:B:726:VAL:HG13	1:B:728:VAL:HG23	2.01	0.43
1:B:195:TYR:CD1	1:B:195:TYR:N	2.86	0.43
1:B:472:CYS:O	1:B:478:PRO:HA	2.19	0.43
1:B:485:SER:O	1:B:486:VAL:C	2.56	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HD22	2.01	0.43
1:B:116:LEU:O	1:B:132:TYR:HA	2.19	0.43
1:B:658:ARG:HH22	1:B:684:ARG:HH21	1.66	0.43
1:B:145:GLU:O	1:B:146:GLU:HB2	2.19	0.43
1:A:512:LYS:HE2	1:A:527:GLN:OE1	2.18	0.42
1:B:202:VAL:HG22	6:B:808:HOH:O	2.18	0.42
1:A:612:GLN:HE21	1:A:612:GLN:HA	1.83	0.42
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.54	0.42
1:B:82:GLU:HB2	1:B:467:TYR:OH	2.19	0.42
1:A:199:THR:OG1	1:A:204:GLU:HB2	2.19	0.42
1:B:597:ARG:HA	1:B:682:HIS:CD2	2.54	0.42
1:B:594:ILE:HD11	1:B:602:GLU:H	1.85	0.42
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.42
1:A:207:VAL:HA	1:A:358:ARG:NH1	2.34	0.42
1:B:109:PRO:HD2	1:B:161:GLY:O	2.19	0.42
1:B:614:SER:O	1:B:615:LYS:C	2.57	0.42
1:A:150:ASN:O	1:A:151:ASN:HB2	2.20	0.42
1:B:177:GLU:HA	1:B:178:PRO:HD3	1.88	0.42
1:A:98:PHE:HE2	1:A:100:HIS:HB2	1.84	0.42
1:B:180:LEU:HD13	1:B:180:LEU:HA	1.74	0.42
1:B:463:LYS:C	1:B:465:ALA:N	2.73	0.42
1:B:603:VAL:HG13	1:B:639:VAL:HG23	2.01	0.42
1:A:528:MET:CE	1:A:530:LEU:HD21	2.45	0.42
1:A:648:LYS:HG2	1:A:762:CYS:SG	2.60	0.42
1:A:139:LYS:O	1:A:140:ARG:C	2.58	0.42
1:A:105:TYR:HA	1:A:115:LEU:O	2.20	0.41
1:B:369:ASN:O	1:B:389:ILE:HG12	2.20	0.41
1:B:433:LYS:HG2	1:B:443:THR:HG23	2.02	0.41
1:B:620:ASP:CG	1:B:622:LYS:HZ1	2.23	0.41
1:B:628:GLY:HA3	1:B:632:GLY:O	2.20	0.41
1:A:513:LYS:HB2	1:A:530:LEU:HD11	2.01	0.41
1:A:612:GLN:HE21	1:A:615:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TRP:CE3	1:B:462:SER:HB3	2.55	0.41
1:B:505:GLN:HE21	1:B:505:GLN:CA	2.29	0.41
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.56	0.41
1:B:759:ILE:HA	1:B:759:ILE:HD13	1.86	0.41
1:A:154:TRP:O	1:A:166:TYR:HA	2.19	0.41
1:B:459:VAL:CG2	1:B:460:SER:N	2.83	0.41
1:B:504:LEU:HA	1:B:507:VAL:HG12	2.03	0.41
1:B:538:LYS:O	1:B:618:PHE:HA	2.20	0.41
1:A:120:TYR:CE1	1:A:128:TYR:CG	3.09	0.41
1:A:330:TYR:CE2	1:A:332:GLU:HG2	2.55	0.41
1:A:248:TYR:HA	1:A:249:PRO:HD3	1.88	0.41
1:B:311:ILE:HG13	1:B:337:TRP:CZ3	2.56	0.41
1:B:658:ARG:HG3	1:B:687:THR:HG22	2.02	0.41
1:B:505:GLN:HA	1:B:505:GLN:NE2	2.31	0.41
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.03	0.41
6:A:960:HOH:O	5:B:1:GOL:H11	2.21	0.41
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.21	0.41
1:A:104:ASP:OD1	1:A:105:TYR:N	2.47	0.40
1:B:498:SER:O	1:B:502:LYS:HE2	2.21	0.40
1:A:237:GLU:OE2	1:A:253:ARG:HD3	2.22	0.40
1:A:518:ILE:HD13	1:A:522:THR:C	2.41	0.40
1:B:658:ARG:NH2	1:B:684:ARG:HE	2.19	0.40
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.56	0.40
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.94	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	725/753 (96%)	680 (94%)	42 (6%)	3 (0%)	38 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/753 (96%)	688 (95%)	37 (5%)	1 (0%)	55	65
All	All	1451/1506 (96%)	1368 (94%)	79 (5%)	4 (0%)	44	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ILE
1	A	146	GLU
1	A	242	SER
1	B	242	SER

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	646/677 (95%)	604 (94%)	42 (6%)	20	22
1	B	646/677 (95%)	597 (92%)	49 (8%)	15	16
All	All	1292/1354 (95%)	1201 (93%)	91 (7%)	18	19

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	59	SER
1	A	77	LEU
1	A	78	VAL
1	A	162	HIS
1	A	180	LEU
1	A	223	LEU
1	A	230	ASP
1	A	243	ASP
1	A	246	LEU
1	A	294	LEU
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	319	ILE
1	A	326	ASP
1	A	350	THR
1	A	366	LEU
1	A	373	LYS
1	A	382	ARG
1	A	410	LEU
1	A	419	SER
1	A	431	LEU
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	486	VAL
1	A	500	LEU
1	A	502	LYS
1	A	513	LYS
1	A	514	LEU
1	A	543	LEU
1	A	544	LEU
1	A	589	LYS
1	A	594	ILE
1	A	627	TRP
1	A	630	SER
1	A	663	ASP
1	A	677	GLU
1	A	696	LYS
1	A	704	HIS
1	A	715	GLN
1	A	736	THR
1	B	42	THR
1	B	61	ARG
1	B	63	ILE
1	B	90	LEU
1	B	94	THR
1	B	104	ASP
1	B	143	ILE
1	B	155	VAL
1	B	156	THR
1	B	202	VAL
1	B	214	LEU
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	230	ASP
1	B	232	GLU
1	B	236	ILE
1	B	246	LEU
1	B	278	SER
1	B	311	ILE
1	B	326	ASP
1	B	327	ILE
1	B	336	ARG
1	B	350	THR
1	B	385	CYS
1	B	393	ASP
1	B	397	ILE
1	B	441	LYS
1	B	443	THR
1	B	463	LYS
1	B	471	ARG
1	B	472	CYS
1	B	479	LEU
1	B	486	VAL
1	B	500	LEU
1	B	505	GLN
1	B	514	LEU
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	597	ARG
1	B	619	VAL
1	B	680	LEU
1	B	684	ARG
1	B	704	HIS
1	B	726	VAL
1	B	745	SER
1	B	764	SER

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

Mol	Chain	Res	Type
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	247	GLN
1	A	281	ASN
1	A	314	GLN
1	A	508	GLN
1	A	533	HIS
1	A	592	HIS
1	A	612	GLN
1	A	697	GLN
1	A	715	GLN
1	A	748	HIS
1	B	169	ASN
1	B	383	HIS
1	B	505	GLN
1	B	562	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 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	2291	1,3	14,14,15	0.55	0	15,19,21	0.58	0
3	NAG	A	2292	3	14,14,15	0.45	0	15,19,21	1.28	1 (6%)
3	NAG	B	2291	1,3	14,14,15	0.57	0	15,19,21	1.34	2 (13%)
3	NAG	B	2292	3	14,14,15	0.70	1 (7%)	15,19,21	2.01	5 (33%)

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	2291	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2292	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2291	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2292	3	-	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	2292	NAG	O5-C1	-2.02	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2292	NAG	O5-C1-C2	-5.46	103.88	111.47
3	B	2291	NAG	C2-N2-C7	-3.19	118.29	122.94
3	B	2292	NAG	C2-N2-C7	-2.22	119.70	122.94
3	B	2291	NAG	O5-C1-C2	-2.08	108.58	111.47
3	B	2292	NAG	C1-O5-C5	-2.04	109.36	112.17
3	B	2292	NAG	C4-C3-C2	2.32	114.42	111.02
3	B	2292	NAG	C3-C4-C5	3.13	115.73	110.22
3	A	2292	NAG	C1-O5-C5	4.09	117.80	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

13 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	$\# Z > 2$
4	6A5	A	1	-	25,31,31	1.23	3 (12%)	32,45,45	1.34	4 (12%)
2	NAG	A	1501	1	14,14,15	0.49	0	15,19,21	1.39	3 (20%)
2	NAG	A	2191	1	14,14,15	0.56	0	15,19,21	1.22	1 (6%)
2	NAG	A	2811	-	14,14,15	0.58	0	15,19,21	1.52	3 (20%)
2	NAG	A	5201	1	14,14,15	0.45	0	15,19,21	1.26	2 (13%)
2	NAG	A	851	1	14,14,15	0.58	0	15,19,21	0.96	1 (6%)
5	GOL	B	1	-	5,5,5	0.30	0	5,5,5	0.35	0
2	NAG	B	1501	1	14,14,15	0.73	0	15,19,21	1.84	3 (20%)
4	6A5	B	2	-	25,31,31	1.55	5 (20%)	32,45,45	1.77	8 (25%)
2	NAG	B	2191	1	14,14,15	0.64	0	15,19,21	1.04	1 (6%)
2	NAG	B	5201	1	14,14,15	0.60	0	15,19,21	0.99	0
2	NAG	B	851	1	14,14,15	0.52	0	15,19,21	1.30	2 (13%)
2	NAG	B	921	1	14,14,15	0.42	0	15,19,21	0.93	1 (6%)

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
4	6A5	A	1	-	-	0/8/22/22	0/4/4/4
2	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	A	2811	-	-	0/6/23/26	0/1/1/1
2	NAG	A	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
5	GOL	B	1	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1501	1	1/1/5/7	0/6/23/26	0/1/1/1
4	6A5	B	2	-	-	0/8/22/22	0/4/4/4
2	NAG	B	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	B	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	B	851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	921	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	6A5	C19-CL23	-3.50	1.66	1.74
4	B	2	6A5	C8-C10	-3.25	1.44	1.50
4	B	2	6A5	C14-C1	-2.55	1.45	1.48
4	A	1	6A5	C24-C25	2.01	1.58	1.50
4	B	2	6A5	C28-N12	2.08	1.50	1.47
4	A	1	6A5	C2-C3	2.16	1.42	1.39
4	B	2	6A5	C2-C3	2.47	1.43	1.39
4	A	1	6A5	C10-N12	2.77	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	NAG	O5-C1-C2	-5.11	104.36	111.47
4	B	2	6A5	C8-C9-N5	-4.68	103.07	107.85
2	A	2811	NAG	O5-C1-C2	-3.36	106.80	111.47
2	A	1501	NAG	O5-C1-C2	-2.74	107.67	111.47
4	B	2	6A5	C13-C3-N4	-2.60	113.13	116.99
4	A	1	6A5	C8-C9-N5	-2.59	105.21	107.85
4	B	2	6A5	C20-C19-CL23	-2.58	115.92	119.14
4	B	2	6A5	C28-N12-C10	-2.55	114.50	122.77
2	A	2811	NAG	C2-N2-C7	-2.53	119.25	122.94
4	B	2	6A5	O26-C27-C28	-2.49	106.27	111.83
2	B	1501	NAG	C1-O5-C5	-2.37	108.90	112.17
2	B	851	NAG	C2-N2-C7	-2.31	119.58	122.94
4	A	1	6A5	C13-C3-N4	-2.29	113.60	116.99
2	A	851	NAG	O5-C1-C2	-2.16	108.47	111.47
2	A	5201	NAG	C3-C4-C5	2.13	113.96	110.22
2	A	5201	NAG	C1-O5-C5	2.23	115.24	112.17
2	A	1501	NAG	C1-O5-C5	2.37	115.43	112.17
4	B	2	6A5	C28-N12-C24	2.48	117.29	112.61
2	B	921	NAG	C1-O5-C5	2.53	115.65	112.17
4	A	1	6A5	C9-C8-N7	2.58	113.48	109.36
2	A	2191	NAG	C2-N2-C7	2.95	127.25	122.94
2	A	2811	NAG	C3-C4-C5	2.97	115.45	110.22
2	A	1501	NAG	C3-C4-C5	3.00	115.51	110.22
2	B	2191	NAG	C1-O5-C5	3.12	116.46	112.17
4	B	2	6A5	C2-C3-N4	3.29	125.89	122.16
2	B	851	NAG	C1-O5-C5	3.33	116.75	112.17
4	A	1	6A5	C2-C3-N4	3.41	126.03	122.16
2	B	1501	NAG	C4-C3-C2	3.42	116.03	111.02
4	B	2	6A5	C9-C8-N7	3.46	114.89	109.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1501	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	6A5	1	0
2	A	2191	NAG	1	0
2	A	2811	NAG	3	0
5	B	1	GOL	1	0
2	B	2191	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	727/753 (96%)	-0.17	8 (1%) 80 87	27, 40, 65, 78	0
1	B	727/753 (96%)	-0.26	7 (0%) 82 88	26, 38, 59, 78	0
All	All	1454/1506 (96%)	-0.21	15 (1%) 82 88	26, 39, 62, 78	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	5.0
1	A	279	VAL	4.3
1	B	766	PRO	4.2
1	B	278	SER	3.6
1	A	765	LEU	3.0
1	B	90	LEU	2.9
1	A	96	ASP	2.5
1	A	275	SER	2.4
1	A	766	PRO	2.4
1	A	336	ARG	2.3
1	A	277	SER	2.3
1	B	280	THR	2.1
1	B	656	VAL	2.1
1	A	280	THR	2.1
1	B	654	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	2291	14/15	0.91	0.13	0.54	43,54,67,72	0
3	NAG	A	2291	14/15	0.92	0.11	-0.09	41,51,56,60	0
3	NAG	A	2292	14/15	0.83	0.28	-	63,67,73,74	0
3	NAG	B	2292	14/15	0.91	0.25	-	61,71,80,84	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	5201	14/15	0.82	0.33	7.87	58,75,83,87	0
2	NAG	B	5201	14/15	0.83	0.30	7.58	50,62,81,84	0
2	NAG	B	2191	14/15	0.87	0.33	6.87	57,66,72,72	0
2	NAG	A	2191	14/15	0.69	0.34	3.30	70,76,80,82	0
2	NAG	B	1501	14/15	0.82	0.22	3.06	60,74,85,91	0
4	6A5	A	1	28/28	0.90	0.17	-0.03	31,40,49,58	0
4	6A5	B	2	28/28	0.93	0.16	-0.14	30,40,52,61	0
2	NAG	B	851	14/15	0.97	0.08	-1.24	30,39,42,42	0
2	NAG	A	851	14/15	0.97	0.07	-1.78	39,41,45,45	0
5	GOL	B	1	6/6	0.83	0.17	-	43,52,57,64	0
2	NAG	A	2811	14/15	0.86	0.26	-	65,75,79,81	0
2	NAG	A	1501	14/15	0.88	0.17	-	69,75,84,85	0
2	NAG	B	921	14/15	0.86	0.21	-	70,75,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.