Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:52 PM GMT

PDB ID	:	1R1J
Title	:	STRUCTURAL ANALYSIS OF NEPRILYSIN WITH VARIOUS SPECIFIC AND POTENT INHIBITORS
Authors	:	Oefner, C.; Roques, B.P.; Fournie-Zaluski, M.C.; Dale, G.E.
Deposited on	:	2003-09-24
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

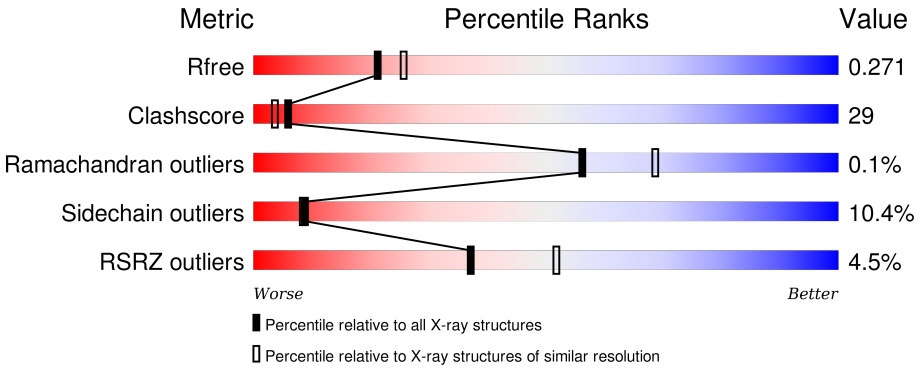
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	696	4% 61% 33% 6%

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
4	OIR	A	2001	-	-	X	-

2 Entry composition

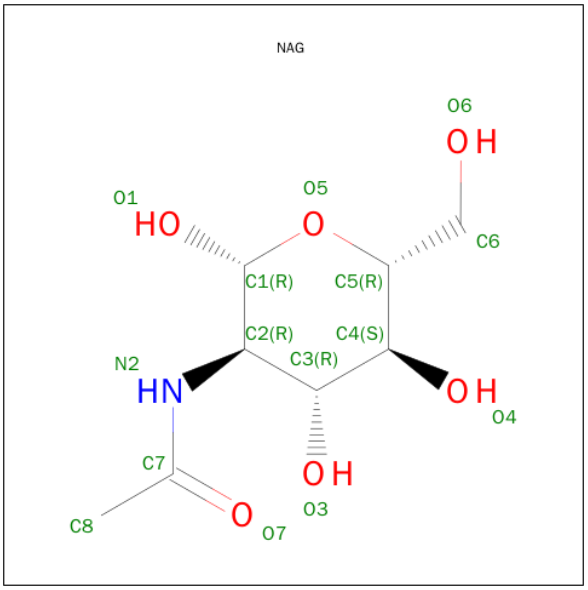
There are 5 unique types of molecules in this entry. The entry contains 5754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neprilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	696	Total	C	N	O	S	0	0	0
			5595	3538	957	1074	26			

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

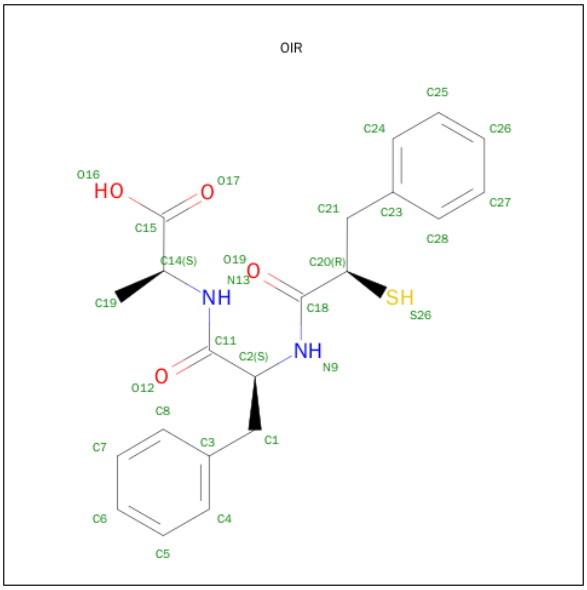


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is N-(3-PHENYL-2-SULFANYLPROPANOYL)PHENYLALANYLALANINE (three-letter code: OIR) (formula: $C_{21}H_{24}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 28	C 21	N 2	O 4	S 1	0	0

- Molecule 5 is water.

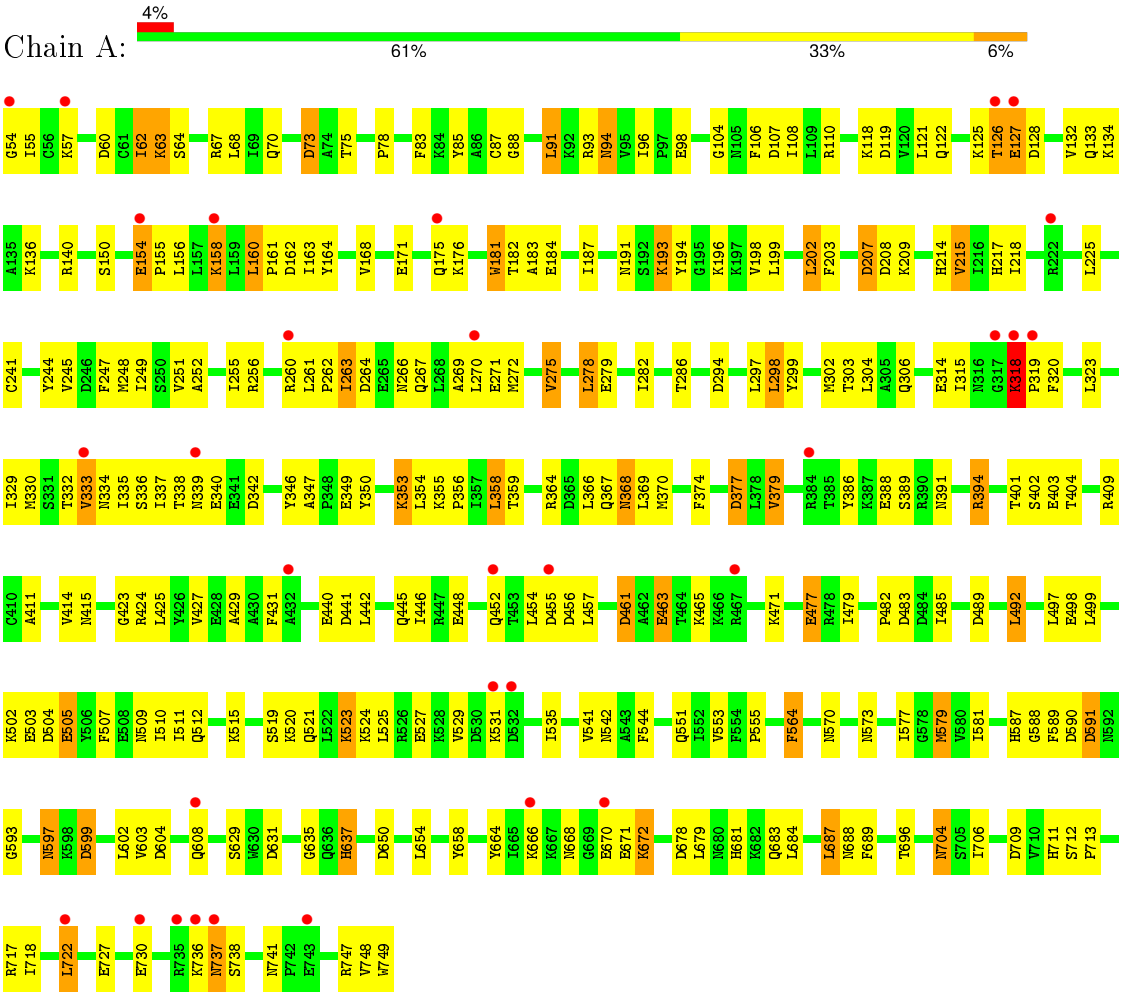
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total 88	O 88	0	0

3 Residue-property plots (i)

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

- Molecule 1: Neprilysin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.46Å 107.46Å 112.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.35 18.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.35) 99.8 (18.98-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.222 , 0.283 0.222 , 0.271	Depositor DCC
R_{free} test set	1585 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.6	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31456 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5754	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, NAG, OIR

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	0.32	0/5713	0.59	20/7727 (0.3%)

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
1	A	0	5

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	604	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	631	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	107	ASP	CB-CG-OD2	5.71	123.43	118.30
1	A	73	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	504	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	207	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	455	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	650	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	678	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	489	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	709	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	591	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	599	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	60	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	461	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	119	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	342	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	456	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	377	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	TRP	Peptide
1	A	429	ALA	Peptide
1	A	431	PHE	Peptide
1	A	564	PHE	Peptide
1	A	737	ASN	Peptide

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	5595	0	5446	318	4
2	A	42	0	39	0	0
3	A	1	0	0	0	0
4	A	28	0	22	14	0
5	A	88	0	0	9	0
All	All	5754	0	5507	319	4

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 29.

All (319) 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:318:LYS:HB3	1:A:319:PRO:C	1.38	1.45
1:A:318:LYS:HB3	1:A:319:PRO:CA	1.55	1.32
1:A:128:ASP:O	1:A:133:GLN:NE2	1.68	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:HD12	1:A:202:LEU:C	1.60	1.19
1:A:303:THR:HG23	1:A:306:GLN:HE21	1.01	1.17
1:A:671:GLU:HB2	1:A:681:HIS:CD2	1.86	1.10
1:A:62:ILE:HD12	1:A:62:ILE:C	1.73	1.09
1:A:278:LEU:O	1:A:282:ILE:HD12	1.54	1.08
1:A:214:HIS:CD2	1:A:524:LYS:HB3	1.90	1.05
1:A:349:GLU:HG3	5:A:2063:HOH:O	1.56	1.04
1:A:689:PHE:HE1	1:A:722:LEU:HD21	1.23	1.03
1:A:158:LYS:HE2	1:A:158:LYS:HA	1.39	1.00
1:A:318:LYS:CB	1:A:319:PRO:CA	2.38	0.99
1:A:318:LYS:CB	1:A:319:PRO:C	2.30	0.99
1:A:202:LEU:CD1	1:A:202:LEU:C	2.28	0.98
1:A:272:MET:O	1:A:275:VAL:HG13	1.64	0.98
1:A:318:LYS:HB3	1:A:319:PRO:HA	1.46	0.97
1:A:579:MET:HE3	4:A:2001:OIR:H7	1.48	0.96
1:A:94:ASN:OD1	5:A:2076:HOH:O	1.82	0.96
1:A:106:PHE:HE2	1:A:110:ARG:HH21	1.08	0.95
1:A:106:PHE:CE2	1:A:110:ARG:NH2	2.35	0.95
1:A:202:LEU:HD12	1:A:203:PHE:N	1.82	0.93
1:A:355:LYS:HB3	1:A:356:PRO:HD3	1.51	0.93
1:A:106:PHE:HE2	1:A:110:ARG:NH2	1.68	0.93
1:A:579:MET:CE	4:A:2001:OIR:H7	1.99	0.92
1:A:333:VAL:HG22	1:A:333:VAL:O	1.69	0.91
1:A:303:THR:HG23	1:A:306:GLN:NE2	1.85	0.91
1:A:718:ILE:O	1:A:722:LEU:HG	1.71	0.91
1:A:318:LYS:CB	1:A:319:PRO:HA	2.00	0.88
1:A:333:VAL:CG2	1:A:333:VAL:O	2.20	0.88
1:A:62:ILE:HD12	1:A:62:ILE:O	1.71	0.87
1:A:748:VAL:HG22	1:A:749:TRP:H	1.40	0.87
1:A:671:GLU:HB2	1:A:681:HIS:HD2	1.39	0.86
1:A:579:MET:HE3	4:A:2001:OIR:C7	2.05	0.86
1:A:336:SER:C	1:A:337:ILE:HD13	1.96	0.86
1:A:366:LEU:C	1:A:370:MET:HE2	1.96	0.85
1:A:214:HIS:NE2	1:A:524:LYS:HD2	1.91	0.85
1:A:597:ASN:ND2	1:A:599:ASP:H	1.73	0.85
1:A:202:LEU:CD1	1:A:203:PHE:N	2.37	0.84
1:A:597:ASN:HD22	1:A:597:ASN:C	1.81	0.84
1:A:689:PHE:CE1	1:A:722:LEU:HD21	2.10	0.84
1:A:333:VAL:HG22	1:A:335:ILE:CD1	2.06	0.83
1:A:579:MET:CE	4:A:2001:OIR:C7	2.57	0.83
1:A:440:GLU:HG2	1:A:479:ILE:CD1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:THR:HG23	1:A:409:ARG:CG	2.10	0.81
1:A:62:ILE:CD1	1:A:62:ILE:C	2.49	0.81
1:A:202:LEU:HB2	1:A:218:ILE:CD1	2.11	0.80
1:A:336:SER:O	1:A:337:ILE:HD13	1.80	0.80
1:A:55:ILE:N	1:A:55:ILE:HD13	1.96	0.80
1:A:748:VAL:CG2	1:A:749:TRP:N	2.44	0.80
1:A:214:HIS:HE1	1:A:529:VAL:HG22	1.47	0.79
1:A:748:VAL:HG22	1:A:749:TRP:N	1.96	0.79
1:A:214:HIS:CE1	1:A:529:VAL:HG22	2.16	0.79
1:A:333:VAL:HG22	1:A:335:ILE:HD12	1.64	0.79
1:A:154:GLU:HG3	1:A:155:PRO:HD3	1.63	0.79
1:A:67:ARG:HH22	1:A:688:ASN:HD21	1.30	0.79
1:A:272:MET:HA	1:A:275:VAL:CG1	2.13	0.79
1:A:366:LEU:HB3	1:A:370:MET:HE1	1.64	0.78
1:A:168:VAL:H	1:A:368:ASN:HD21	1.32	0.78
1:A:404:THR:CG2	1:A:409:ARG:HG2	2.13	0.77
1:A:302:MET:HG2	1:A:306:GLN:HB2	1.66	0.77
1:A:73:ASP:OD1	1:A:75:THR:OG1	2.02	0.77
1:A:440:GLU:CG	1:A:479:ILE:CD1	2.64	0.76
1:A:440:GLU:HG2	1:A:479:ILE:HD12	1.67	0.76
1:A:629:SER:HB2	1:A:635:GLY:O	1.85	0.76
1:A:67:ARG:HH22	1:A:688:ASN:ND2	1.84	0.75
1:A:507:PHE:O	1:A:510:ILE:HG12	1.85	0.75
1:A:87:CYS:O	1:A:91:LEU:HD22	1.87	0.74
1:A:551:GLN:HE21	1:A:553:VAL:CG2	2.00	0.74
1:A:333:VAL:CG2	1:A:335:ILE:CD1	2.65	0.74
1:A:214:HIS:CD2	1:A:524:LYS:CB	2.70	0.73
1:A:355:LYS:HB3	1:A:356:PRO:CD	2.18	0.73
1:A:394:ARG:HH21	1:A:402:SER:N	1.88	0.72
1:A:207:ASP:HB2	1:A:215:VAL:HG22	1.71	0.72
1:A:681:HIS:ND1	1:A:684:LEU:HD12	2.04	0.71
1:A:588:GLY:O	1:A:593:GLY:O	2.09	0.71
1:A:78:PRO:HG3	1:A:85:TYR:CD1	2.25	0.71
1:A:507:PHE:O	1:A:510:ILE:CG1	2.39	0.71
1:A:333:VAL:CG2	1:A:335:ILE:HD12	2.20	0.70
1:A:411:ALA:O	1:A:414:VAL:HG22	1.91	0.70
1:A:404:THR:HG23	1:A:409:ARG:HG2	1.72	0.70
1:A:579:MET:CE	4:A:2001:OIR:C6	2.70	0.70
1:A:527:GLU:OE1	5:A:2039:HOH:O	2.09	0.70
1:A:245:VAL:O	1:A:249:ILE:HG13	1.91	0.70
1:A:68:LEU:HD22	1:A:687:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:CE	1:A:158:LYS:HA	2.19	0.69
1:A:154:GLU:N	1:A:155:PRO:CD	2.56	0.69
1:A:202:LEU:O	1:A:202:LEU:HD12	1.92	0.68
1:A:722:LEU:HD23	1:A:722:LEU:N	2.08	0.68
1:A:535:ILE:HG12	1:A:551:GLN:NE2	2.08	0.67
1:A:278:LEU:HD22	1:A:282:ILE:HD11	1.77	0.67
1:A:366:LEU:O	1:A:370:MET:HE2	1.93	0.67
1:A:67:ARG:NH2	1:A:688:ASN:HD21	1.93	0.67
1:A:67:ARG:HH12	1:A:688:ASN:ND2	1.93	0.66
1:A:78:PRO:HG3	1:A:85:TYR:CE1	2.31	0.66
1:A:367:GLN:HA	1:A:370:MET:HE3	1.79	0.64
1:A:579:MET:CE	4:A:2001:OIR:H6	2.26	0.64
1:A:333:VAL:CG2	1:A:335:ILE:HD11	2.28	0.64
1:A:106:PHE:CE2	1:A:541:VAL:O	2.50	0.64
1:A:126:THR:HG22	1:A:127:GLU:OE2	1.98	0.64
1:A:67:ARG:HH12	1:A:688:ASN:HD22	1.43	0.64
1:A:193:LYS:CD	1:A:515:LYS:HE2	2.28	0.64
1:A:318:LYS:HB3	1:A:319:PRO:O	1.97	0.64
1:A:542:ASN:O	1:A:555:PRO:HD2	1.99	0.63
1:A:202:LEU:HD13	1:A:203:PHE:N	2.14	0.63
1:A:303:THR:CG2	1:A:306:GLN:HE21	1.94	0.63
1:A:403:GLU:HG3	5:A:2050:HOH:O	1.97	0.62
1:A:713:PRO:HG3	5:A:2041:HOH:O	1.96	0.62
1:A:577:ILE:O	1:A:581:ILE:HG13	1.99	0.62
1:A:404:THR:HG23	1:A:409:ARG:HG3	1.81	0.62
1:A:440:GLU:CG	1:A:479:ILE:HD12	2.27	0.62
1:A:209:LYS:HE3	1:A:299:TYR:CD1	2.35	0.62
1:A:366:LEU:HB3	1:A:370:MET:CE	2.30	0.62
1:A:579:MET:HE1	4:A:2001:OIR:H7	1.80	0.61
1:A:689:PHE:HE1	1:A:722:LEU:CD2	2.07	0.61
1:A:225:LEU:HD21	1:A:244:TYR:CG	2.36	0.61
1:A:366:LEU:C	1:A:370:MET:CE	2.69	0.61
1:A:748:VAL:CG2	1:A:749:TRP:CD1	2.84	0.61
1:A:193:LYS:O	1:A:515:LYS:HG2	2.02	0.59
1:A:193:LYS:HD2	1:A:515:LYS:HE2	1.82	0.59
1:A:579:MET:HE1	4:A:2001:OIR:H6	1.83	0.59
1:A:597:ASN:HD22	1:A:599:ASP:H	1.46	0.59
1:A:379:VAL:HG22	1:A:386:TYR:HB3	1.85	0.59
1:A:570:ASN:ND2	1:A:664:TYR:OH	2.36	0.59
1:A:140:ARG:HH21	1:A:503:GLU:CD	2.05	0.59
1:A:354:LEU:HG	1:A:358:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:NH2	1:A:402:SER:N	2.49	0.58
1:A:202:LEU:HB2	1:A:218:ILE:HD13	1.82	0.58
1:A:267:GLN:NE2	1:A:270:LEU:HD23	2.18	0.58
1:A:689:PHE:CE1	1:A:722:LEU:CD2	2.85	0.58
1:A:448:GLU:OE2	1:A:452:GLN:NE2	2.36	0.58
1:A:414:VAL:HG23	1:A:415:ASN:N	2.19	0.58
1:A:160:LEU:HD12	1:A:163:ILE:HD11	1.84	0.58
1:A:579:MET:HE1	4:A:2001:OIR:C7	2.32	0.57
1:A:209:LYS:HD2	1:A:299:TYR:CE1	2.38	0.57
1:A:404:THR:CG2	1:A:409:ARG:CG	2.77	0.57
1:A:182:THR:OG1	1:A:184:GLU:HG2	2.05	0.57
1:A:535:ILE:CG1	1:A:553:VAL:HG21	2.35	0.56
1:A:597:ASN:ND2	1:A:597:ASN:C	2.50	0.56
1:A:507:PHE:HA	1:A:510:ILE:CD1	2.34	0.56
1:A:388:GLU:O	1:A:391:ASN:ND2	2.38	0.56
1:A:461:ASP:OD2	1:A:463:GLU:HG2	2.05	0.56
1:A:278:LEU:HD13	1:A:369:LEU:CD2	2.36	0.56
1:A:247:PHE:HE2	1:A:389:SER:HG	1.53	0.56
1:A:564:PHE:HA	1:A:573:ASN:OD1	2.05	0.56
1:A:126:THR:CG2	1:A:127:GLU:OE2	2.53	0.56
1:A:163:ILE:O	1:A:164:TYR:HB2	2.05	0.56
1:A:214:HIS:CE1	1:A:529:VAL:CG2	2.87	0.56
1:A:261:LEU:HB3	1:A:262:PRO:HD2	1.86	0.56
1:A:154:GLU:HG3	1:A:155:PRO:CD	2.33	0.55
1:A:160:LEU:N	1:A:161:PRO:CD	2.69	0.55
1:A:278:LEU:HD13	1:A:369:LEU:HD23	1.88	0.55
1:A:579:MET:HE1	4:A:2001:OIR:C6	2.33	0.55
1:A:333:VAL:HG13	1:A:335:ILE:HD12	1.88	0.55
1:A:394:ARG:HH21	1:A:401:THR:C	2.08	0.55
1:A:162:ASP:OD1	1:A:193:LYS:HE2	2.07	0.55
1:A:249:ILE:HD11	1:A:269:ALA:HA	1.88	0.55
1:A:440:GLU:HG3	1:A:479:ILE:CD1	2.34	0.55
1:A:551:GLN:HE21	1:A:553:VAL:HG21	1.71	0.55
1:A:106:PHE:CE2	1:A:110:ARG:CZ	2.90	0.55
1:A:62:ILE:CD1	1:A:62:ILE:O	2.49	0.54
1:A:440:GLU:HG3	1:A:479:ILE:HD13	1.88	0.54
1:A:279:GLU:HA	1:A:282:ILE:HD13	1.89	0.54
1:A:333:VAL:CG1	1:A:335:ILE:HD12	2.38	0.54
1:A:132:VAL:HG22	1:A:425:LEU:HD11	1.88	0.54
1:A:349:GLU:O	1:A:353:LYS:HD3	2.08	0.54
1:A:171:GLU:CG	1:A:176:LYS:HE2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD22	1:A:282:ILE:CD1	2.38	0.54
1:A:502:LYS:H	1:A:509:ASN:HD21	1.55	0.54
1:A:196:LYS:HE3	1:A:374:PHE:HA	1.91	0.53
1:A:403:GLU:HG2	1:A:409:ARG:HD3	1.89	0.53
1:A:423:GLY:O	1:A:427:VAL:HG22	2.08	0.53
1:A:367:GLN:CA	1:A:370:MET:HE3	2.38	0.53
1:A:73:ASP:OD2	1:A:75:THR:OG1	2.27	0.53
1:A:713:PRO:HD3	5:A:2041:HOH:O	2.09	0.53
1:A:181:TRP:O	1:A:182:THR:HG22	2.08	0.53
1:A:171:GLU:O	1:A:176:LYS:CD	2.57	0.53
1:A:214:HIS:HD2	1:A:524:LYS:CB	2.21	0.53
1:A:62:ILE:HD12	1:A:63:LYS:N	2.21	0.53
1:A:271:GLU:OE1	1:A:364:ARG:NH2	2.42	0.53
1:A:121:LEU:CD1	1:A:414:VAL:HG21	2.39	0.52
1:A:241:CYS:O	1:A:245:VAL:HG23	2.09	0.52
1:A:654:LEU:HD13	1:A:689:PHE:CD2	2.44	0.52
1:A:333:VAL:HG21	1:A:335:ILE:HD11	1.89	0.52
1:A:679:LEU:HA	1:A:683:GLN:OE1	2.09	0.52
1:A:535:ILE:HG12	1:A:551:GLN:HE21	1.74	0.52
1:A:337:ILE:HD13	1:A:337:ILE:N	2.23	0.52
1:A:202:LEU:HB2	1:A:218:ILE:HD11	1.90	0.52
1:A:404:THR:HG22	5:A:2050:HOH:O	2.10	0.52
1:A:671:GLU:HB2	1:A:681:HIS:NE2	2.21	0.52
1:A:181:TRP:CE3	1:A:182:THR:HA	2.44	0.52
1:A:171:GLU:HG2	1:A:176:LYS:HE2	1.92	0.51
1:A:247:PHE:O	1:A:251:VAL:HG23	2.10	0.51
1:A:502:LYS:HB2	1:A:505:GLU:HB2	1.93	0.51
1:A:507:PHE:O	1:A:510:ILE:HG13	2.11	0.51
1:A:271:GLU:O	1:A:275:VAL:HG12	2.11	0.51
1:A:272:MET:HA	1:A:275:VAL:HG12	1.91	0.51
1:A:198:VAL:O	1:A:199:LEU:HB2	2.11	0.51
1:A:154:GLU:N	1:A:155:PRO:HD3	2.26	0.51
1:A:323:LEU:HD22	1:A:339:ASN:OD1	2.11	0.51
1:A:737:ASN:N	1:A:741:ASN:O	2.43	0.51
1:A:318:LYS:HG3	1:A:319:PRO:O	2.10	0.50
1:A:507:PHE:HA	1:A:510:ILE:HD11	1.92	0.50
1:A:73:ASP:CG	1:A:75:THR:OG1	2.48	0.50
1:A:249:ILE:CD1	1:A:269:ALA:HA	2.41	0.50
1:A:394:ARG:NH2	1:A:401:THR:C	2.65	0.50
1:A:587:HIS:CD2	4:A:2001:OIR:S26	3.05	0.50
1:A:704:ASN:HD22	1:A:704:ASN:C	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:MET:C	1:A:275:VAL:HG13	2.30	0.50
1:A:318:LYS:HB3	1:A:320:PHE:N	2.18	0.49
1:A:214:HIS:HE1	1:A:529:VAL:CG2	2.22	0.49
1:A:315:ILE:CD1	1:A:320:PHE:CD2	2.96	0.49
1:A:629:SER:HB3	1:A:637:HIS:CE1	2.46	0.49
1:A:411:ALA:O	1:A:414:VAL:CG2	2.60	0.49
1:A:711:HIS:HE2	4:A:2001:OIR:C18	2.25	0.49
1:A:712:SER:O	1:A:717:ARG:HD2	2.13	0.49
1:A:535:ILE:HG12	1:A:553:VAL:HG21	1.94	0.48
1:A:54:GLY:O	1:A:672:LYS:HD3	2.13	0.48
1:A:279:GLU:HA	1:A:282:ILE:CD1	2.44	0.48
1:A:271:GLU:CD	1:A:364:ARG:HH21	2.17	0.48
1:A:664:TYR:CD2	1:A:668:ASN:ND2	2.81	0.48
1:A:244:TYR:O	1:A:248:MET:HG3	2.13	0.48
1:A:183:ALA:HB2	1:A:315:ILE:HG21	1.96	0.47
1:A:366:LEU:CB	1:A:370:MET:HE1	2.39	0.47
1:A:98:GLU:HB3	1:A:401:THR:OG1	2.14	0.47
1:A:70:GLN:HG2	1:A:93:ARG:HH12	1.79	0.47
1:A:106:PHE:HE2	1:A:110:ARG:CZ	2.25	0.47
1:A:347:ALA:HB1	1:A:350:TYR:HB3	1.96	0.47
1:A:523:LYS:O	1:A:523:LYS:HG3	2.14	0.47
1:A:96:ILE:HD11	1:A:696:THR:HG23	1.95	0.47
1:A:507:PHE:C	1:A:510:ILE:HG12	2.34	0.47
1:A:251:VAL:O	1:A:255:ILE:HG13	2.14	0.47
1:A:477:GLU:O	1:A:477:GLU:HG2	2.14	0.47
1:A:303:THR:H	1:A:306:GLN:HG3	1.80	0.47
1:A:202:LEU:HD12	1:A:203:PHE:CA	2.44	0.46
1:A:121:LEU:HD13	1:A:414:VAL:HG21	1.98	0.46
1:A:394:ARG:NH2	1:A:402:SER:CA	2.78	0.46
1:A:196:LYS:NZ	1:A:377:ASP:OD1	2.46	0.46
1:A:736:LYS:O	1:A:738:SER:N	2.48	0.46
1:A:544:PHE:CE1	4:A:2001:OIR:H24	2.51	0.46
1:A:67:ARG:NH1	1:A:688:ASN:ND2	2.63	0.46
1:A:424:ARG:HD2	1:A:485:ILE:O	2.15	0.46
1:A:404:THR:HG21	1:A:409:ARG:HG2	1.96	0.46
1:A:367:GLN:HA	1:A:370:MET:CE	2.43	0.46
1:A:106:PHE:HE2	1:A:541:VAL:O	1.94	0.46
1:A:670:GLU:HG3	1:A:671:GLU:N	2.31	0.45
1:A:713:PRO:CG	5:A:2041:HOH:O	2.62	0.45
1:A:247:PHE:HE2	1:A:389:SER:OG	1.98	0.45
1:A:330:MET:C	1:A:332:THR:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:CA	1:A:158:LYS:HE2	2.27	0.45
1:A:294:ASP:CG	1:A:297:LEU:HG	2.36	0.45
1:A:252:ALA:O	1:A:256:ARG:HG3	2.16	0.45
4:A:2001:OIR:H28	4:A:2001:OIR:H20	1.39	0.45
1:A:263:ILE:O	1:A:263:ILE:HG22	2.16	0.45
1:A:597:ASN:HD21	1:A:599:ASP:HB2	1.82	0.45
1:A:272:MET:CA	1:A:275:VAL:CG1	2.91	0.45
1:A:215:VAL:HG23	1:A:217:HIS:CE1	2.52	0.45
1:A:722:LEU:CD2	1:A:722:LEU:N	2.78	0.44
1:A:354:LEU:HG	1:A:358:LEU:CD2	2.46	0.44
1:A:134:LYS:NZ	1:A:499:LEU:O	2.45	0.44
1:A:264:ASP:OD1	1:A:264:ASP:C	2.56	0.44
1:A:524:LYS:O	1:A:525:LEU:C	2.56	0.44
1:A:181:TRP:O	1:A:182:THR:CG2	2.66	0.44
1:A:315:ILE:HD12	1:A:320:PHE:CD2	2.52	0.44
1:A:521:GLN:HA	1:A:521:GLN:OE1	2.17	0.44
1:A:282:ILE:O	1:A:286:THR:HG23	2.18	0.44
1:A:171:GLU:HG3	1:A:176:LYS:HE2	2.00	0.44
1:A:315:ILE:HG23	1:A:366:LEU:CD1	2.48	0.44
1:A:83:PHE:O	1:A:87:CYS:HB2	2.17	0.44
1:A:193:LYS:HG2	1:A:194:TYR:CE2	2.52	0.44
1:A:132:VAL:HG13	1:A:136:LYS:HE3	1.99	0.44
1:A:104:GLY:O	1:A:108:ILE:HG13	2.18	0.43
1:A:171:GLU:O	1:A:176:LYS:HE2	2.17	0.43
1:A:202:LEU:HG	1:A:329:ILE:HD13	2.00	0.43
1:A:127:GLU:H	1:A:127:GLU:HG2	1.54	0.43
1:A:499:LEU:HD23	1:A:512:GLN:OE1	2.19	0.43
1:A:414:VAL:CG2	1:A:415:ASN:N	2.82	0.43
1:A:333:VAL:HG23	1:A:333:VAL:O	2.15	0.43
1:A:457:LEU:O	1:A:465:LYS:NZ	2.39	0.43
1:A:303:THR:OG1	1:A:306:GLN:HG3	2.18	0.43
1:A:507:PHE:HA	1:A:510:ILE:HG12	2.01	0.43
1:A:440:GLU:CG	1:A:479:ILE:HD13	2.45	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.82	0.42
1:A:718:ILE:HG23	1:A:722:LEU:HD11	2.01	0.42
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.90	0.42
1:A:168:VAL:O	1:A:168:VAL:HG22	2.19	0.42
1:A:54:GLY:C	1:A:672:LYS:HD3	2.40	0.42
1:A:424:ARG:HB2	1:A:485:ILE:HG13	2.00	0.42
1:A:507:PHE:CD2	1:A:510:ILE:HD11	2.54	0.42
1:A:315:ILE:HG23	1:A:366:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:O	1:A:445:GLN:HG3	2.19	0.42
1:A:591:ASP:OD1	1:A:591:ASP:N	2.52	0.42
1:A:154:GLU:C	1:A:154:GLU:CD	2.78	0.42
1:A:590:ASP:C	1:A:590:ASP:OD1	2.57	0.42
1:A:658:TYR:CE2	1:A:727:GLU:HG2	2.55	0.42
1:A:570:ASN:ND2	1:A:671:GLU:OE2	2.53	0.42
1:A:589:PHE:HB3	1:A:749:TRP:CZ2	2.55	0.42
1:A:454:LEU:O	1:A:465:LYS:HD3	2.19	0.42
1:A:367:GLN:N	1:A:370:MET:CE	2.82	0.41
1:A:318:LYS:CE	1:A:318:LYS:HA	2.43	0.41
1:A:278:LEU:C	1:A:282:ILE:HD12	2.33	0.41
1:A:736:LYS:C	1:A:738:SER:H	2.24	0.41
1:A:333:VAL:HG21	1:A:335:ILE:CD1	2.44	0.41
1:A:106:PHE:CZ	1:A:541:VAL:O	2.73	0.41
1:A:118:LYS:O	1:A:122:GLN:HG2	2.20	0.41
1:A:88:GLY:HA2	1:A:91:LEU:HD23	2.01	0.41
1:A:298:LEU:HD13	1:A:346:TYR:CD1	2.55	0.41
1:A:511:ILE:HA	1:A:511:ILE:HD13	1.88	0.41
1:A:183:ALA:O	1:A:187:ILE:HD12	2.21	0.41
1:A:570:ASN:ND2	1:A:664:TYR:CZ	2.89	0.41
1:A:214:HIS:NE2	1:A:524:LYS:CD	2.75	0.41
1:A:140:ARG:NE	1:A:503:GLU:OE2	2.39	0.41
1:A:294:ASP:OD2	1:A:297:LEU:HG	2.20	0.41
1:A:191:ASN:OD1	1:A:191:ASN:C	2.59	0.41
1:A:366:LEU:CB	1:A:370:MET:CE	2.99	0.40
1:A:121:LEU:HD11	1:A:414:VAL:HG21	2.03	0.40
1:A:318:LYS:HD2	1:A:318:LYS:HA	1.56	0.40
1:A:256:ARG:NH1	1:A:262:PRO:O	2.53	0.40
1:A:713:PRO:CD	5:A:2041:HOH:O	2.69	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLN:OE1	1:A:260:ARG:C[6_555]	1.46	0.74
1:A:175:GLN:OE1	1:A:260:ARG:O[6_555]	1.48	0.72
1:A:175:GLN:OE1	1:A:261:LEU:N[6_555]	2.01	0.19
1:A:171:GLU:CG	1:A:171:GLU:OE2[6_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	694/696 (100%)	666 (96%)	27 (4%)	1 (0%)	56 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	LYS

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	605/605 (100%)	542 (90%)	63 (10%)	9 8

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	62	ILE
1	A	63	LYS
1	A	64	SER
1	A	91	LEU
1	A	94	ASN
1	A	125	LYS
1	A	126	THR
1	A	127	GLU
1	A	150	SER

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Mol	Chain	Res	Type
1	A	154	GLU
1	A	156	LEU
1	A	158	LYS
1	A	160	LEU
1	A	193	LYS
1	A	202	LEU
1	A	215	VAL
1	A	263	ILE
1	A	266	ASN
1	A	275	VAL
1	A	278	LEU
1	A	298	LEU
1	A	314	GLU
1	A	318	LYS
1	A	333	VAL
1	A	334	ASN
1	A	338	THR
1	A	340	GLU
1	A	353	LYS
1	A	358	LEU
1	A	359	THR
1	A	368	ASN
1	A	379	VAL
1	A	394	ARG
1	A	442	LEU
1	A	446	ILE
1	A	463	GLU
1	A	471	LYS
1	A	477	GLU
1	A	482	PRO
1	A	483	ASP
1	A	492	LEU
1	A	497	LEU
1	A	498	GLU
1	A	505	GLU
1	A	519	SER
1	A	520	LYS
1	A	523	LYS
1	A	531	LYS
1	A	579	MET
1	A	597	ASN
1	A	602	LEU

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Mol	Chain	Res	Type
1	A	603	VAL
1	A	608	GLN
1	A	637	HIS
1	A	666	LYS
1	A	672	LYS
1	A	687	LEU
1	A	704	ASN
1	A	706	ILE
1	A	722	LEU
1	A	730	GLU
1	A	747	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	267	GLN
1	A	306	GLN
1	A	316	ASN
1	A	368	ASN
1	A	391	ASN
1	A	490	ASN
1	A	509	ASN
1	A	550	ASN
1	A	551	GLN
1	A	570	ASN
1	A	597	ASN
1	A	617	GLN
1	A	619	GLN
1	A	656	GLN
1	A	688	ASN
1	A	704	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	OIR	A	2001	3	25,29,29	0.58	1 (4%)	30,38,38	1.13	3 (10%)
2	NAG	A	752	1	14,14,15	0.55	0	15,19,21	0.80	0
2	NAG	A	753	1	14,14,15	0.62	0	15,19,21	0.68	0
2	NAG	A	754	1	14,14,15	0.52	0	15,19,21	0.87	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	OIR	A	2001	3	-	0/22/28/28	0/2/2/2
2	NAG	A	752	1	-	0/6/23/26	0/1/1/1
2	NAG	A	753	1	-	0/6/23/26	0/1/1/1
2	NAG	A	754	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)
4	A	2001	OIR	C20-C18	-2.14	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	OIR	C2-N9-C18	-3.37	114.07	121.62
4	A	2001	OIR	C23-C21-C20	-3.13	107.54	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	OIR	C3-C1-C2	-2.70	105.55	113.41
2	A	754	NAG	C2-N2-C7	-2.21	120.20	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	OIR	14	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	696/696 (100%)	0.27	31 (4%) 37 52	18, 30, 46, 60	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	ARG	3.6
1	A	318	LYS	3.4
1	A	333	VAL	3.3
1	A	260	ARG	3.3
1	A	736	LYS	3.3
1	A	127	GLU	3.2
1	A	126	THR	3.1
1	A	270	LEU	3.1
1	A	319	PRO	2.9
1	A	339	ASN	2.8
1	A	531	LYS	2.7
1	A	666	LYS	2.7
1	A	222	ARG	2.6
1	A	384	ARG	2.5
1	A	432	ALA	2.5
1	A	175	GLN	2.5
1	A	467	ARG	2.5
1	A	608	GLN	2.5
1	A	154	GLU	2.4
1	A	743	GLU	2.4
1	A	737	ASN	2.3
1	A	670	GLU	2.3
1	A	57	LYS	2.3
1	A	317	GLY	2.3
1	A	730	GLU	2.1
1	A	722	LEU	2.1
1	A	452	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLY	2.1
1	A	455	ASP	2.1
1	A	532	ASP	2.1
1	A	158	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	OIR	A	2001	28/28	0.88	0.19	1.58	26,35,52,53	0
2	NAG	A	754	14/15	0.87	0.28	0.87	51,54,57,59	0
2	NAG	A	753	14/15	0.91	0.24	0.47	40,43,47,50	0
3	ZN	A	1001	1/1	0.99	0.02	-5.92	26,26,26,26	0
2	NAG	A	752	14/15	0.84	0.33	-	46,50,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.