Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:25 PM GMT

PDB ID	:	4RZ8
Title	:	Crystal structure of HIV-1 gp120 core in complex with NBD-11021, a small molecule CD4-antagonist
Authors	:	Kwon, Y.D.; Debnath, A.K.; Kwong, P.D.
Deposited on	:	2014-12-18
Resolution	:	1.90 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:

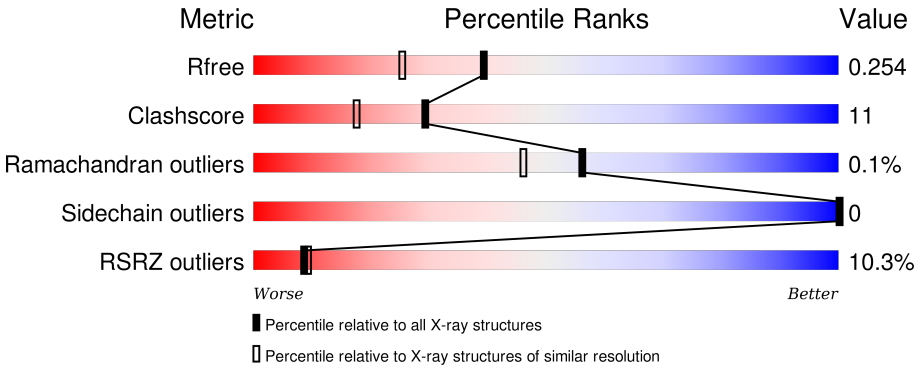
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	353	18% 72% 24% .
1	B	353	14% 74% 21% 5%
1	C	353	4% 75% 21% .
1	D	353	4% 76% 20% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	505	-	-	-	X
2	NAG	A	506	-	-	-	X
2	NAG	B	501	-	-	-	X
2	NAG	B	507	-	-	-	X
2	NAG	B	508	-	-	-	X
2	NAG	C	507	-	-	-	X
2	NAG	C	511	-	-	-	X
2	NAG	D	511	-	-	-	X
3	3ZM	A	510	-	-	-	X
3	3ZM	B	510	-	-	-	X
3	3ZM	D	512	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12111 atoms, of which 100 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	B	334	Total	C	N	O	S	0	0	0
			2617	1645	453	499	20			
1	C	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	D	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			

There are 36 discrepancies between the modelled and reference sequences:

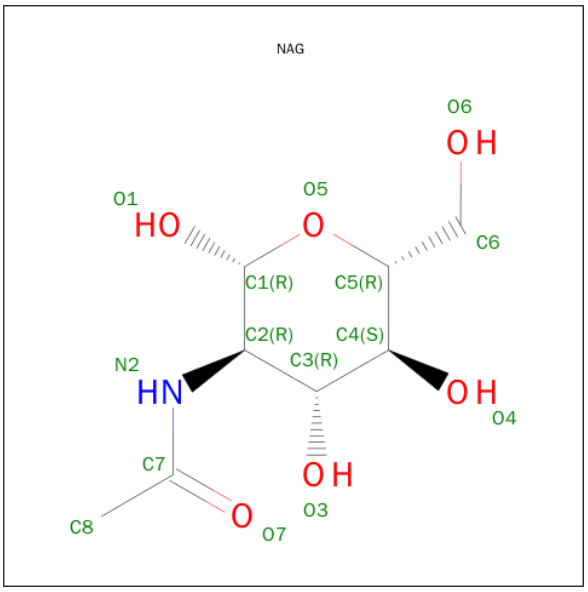
Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	LINKER	UNP Q0ED31
A	198	GLY	-	LINKER	UNP Q0ED31
A	318	GLY	-	LINKER	UNP Q0ED31
A	319	GLY	-	LINKER	UNP Q0ED31
A	320	SER	-	LINKER	UNP Q0ED31
A	321	GLY	-	LINKER	UNP Q0ED31
A	322	SER	-	LINKER	UNP Q0ED31
A	323	GLY	-	LINKER	UNP Q0ED31
A	375	SER	HIS	ENGINEERED MUTATION	UNP Q0ED31
B	124	GLY	-	LINKER	UNP Q0ED31
B	198	GLY	-	LINKER	UNP Q0ED31
B	318	GLY	-	LINKER	UNP Q0ED31
B	319	GLY	-	LINKER	UNP Q0ED31
B	320	SER	-	LINKER	UNP Q0ED31
B	321	GLY	-	LINKER	UNP Q0ED31
B	322	SER	-	LINKER	UNP Q0ED31
B	323	GLY	-	LINKER	UNP Q0ED31
B	375	SER	HIS	ENGINEERED MUTATION	UNP Q0ED31
C	124	GLY	-	LINKER	UNP Q0ED31
C	198	GLY	-	LINKER	UNP Q0ED31
C	318	GLY	-	LINKER	UNP Q0ED31

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	319	GLY	-	LINKER	UNP Q0ED31
C	320	SER	-	LINKER	UNP Q0ED31
C	321	GLY	-	LINKER	UNP Q0ED31
C	322	SER	-	LINKER	UNP Q0ED31
C	323	GLY	-	LINKER	UNP Q0ED31
C	375	SER	HIS	ENGINEERED MUTATION	UNP Q0ED31
D	124	GLY	-	LINKER	UNP Q0ED31
D	198	GLY	-	LINKER	UNP Q0ED31
D	318	GLY	-	LINKER	UNP Q0ED31
D	319	GLY	-	LINKER	UNP Q0ED31
D	320	SER	-	LINKER	UNP Q0ED31
D	321	GLY	-	LINKER	UNP Q0ED31
D	322	SER	-	LINKER	UNP Q0ED31
D	323	GLY	-	LINKER	UNP Q0ED31
D	375	SER	HIS	ENGINEERED MUTATION	UNP Q0ED31

- 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		

Continued on next page...

Continued from previous page...

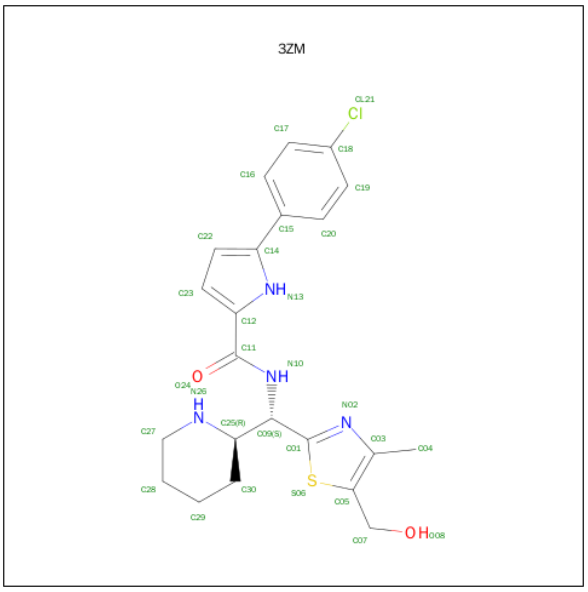
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total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

Continued on next page...

Continued from previous page...

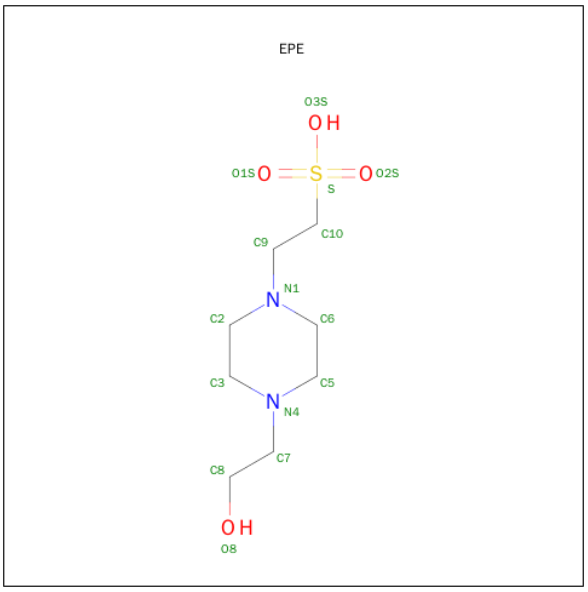
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total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

- Molecule 3 is 5-(4-CHLOROPHENYL)-N-{(S)-[5-(HYDROXYMETHYL)-4-METHYL-1,3-THIAZOL-2-YL][(2R)-PIPERIDIN-2-YL]METHYL}-1H-PYRROLE-2-CARBOXAMIDE (three-letter code: 3ZM) (formula: $C_{22}H_{25}ClN_4O_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	H	N	O	S	0	0
			55	22	1	25	4	2	1		
3	B	1	Total	C	Cl	H	N	O	S	0	0
			55	22	1	25	4	2	1		
3	C	1	Total	C	Cl	H	N	O	S	0	0
			55	22	1	25	4	2	1		
3	D	1	Total	C	Cl	H	N	O	S	0	0
			55	22	1	25	4	2	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

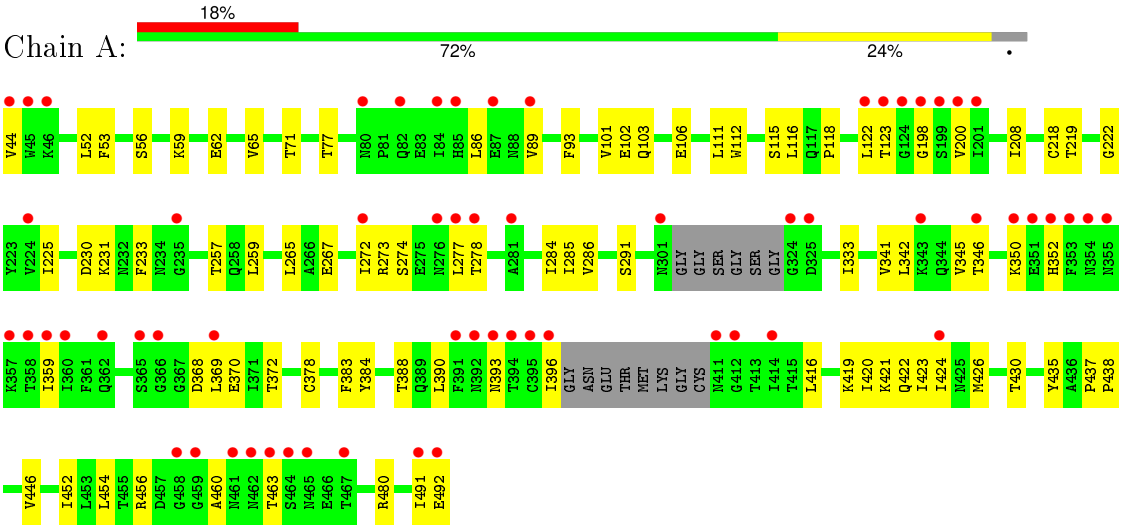
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	126	Total	O	0	0
			126	126		
5	C	232	Total	O	0	0
			232	232		
5	D	242	Total	O	0	0
			242	242		

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.

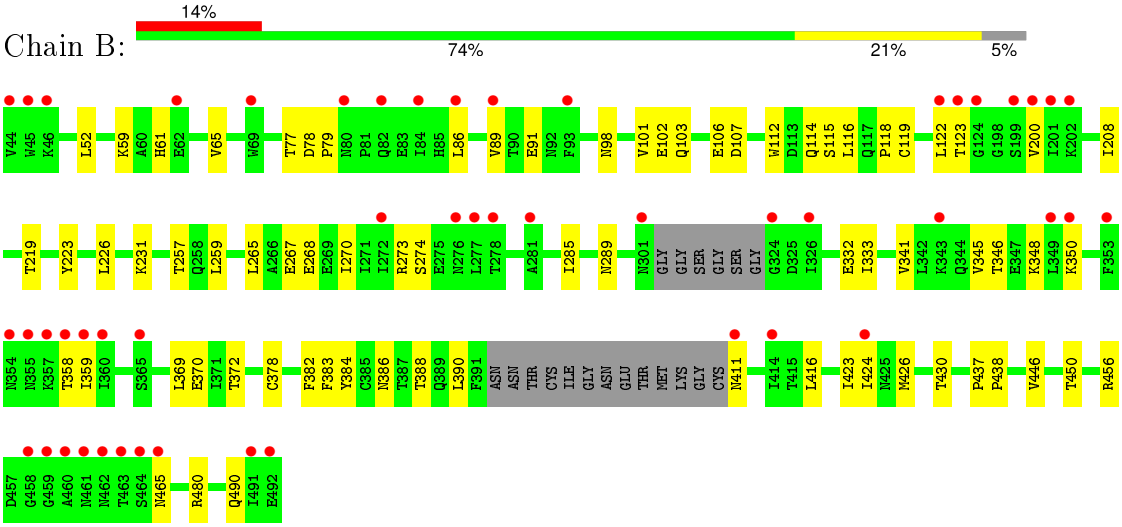
- Molecule 1: Envelope glycoprotein gp120

Chain A:



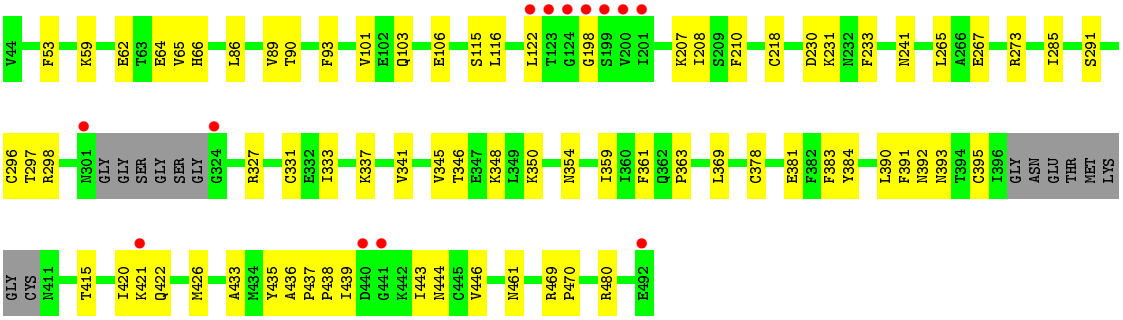
- Molecule 1: Envelope glycoprotein gp120

Chain B:

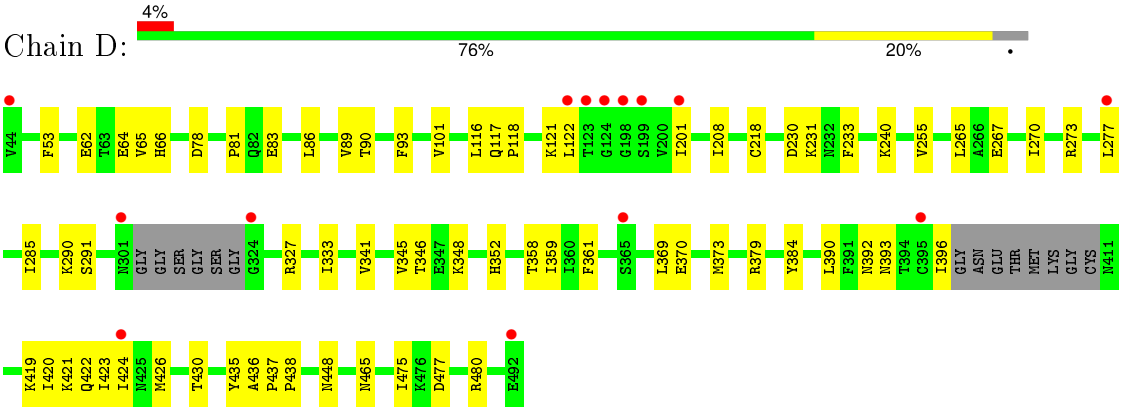


- Molecule 1: Envelope glycoprotein gp120

Chain C:



- Molecule 1: Envelope glycoprotein gp120



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.62Å 68.84Å 116.19Å 90.00° 110.59° 90.00°	Depositor
Resolution (Å)	44.03 – 1.90 44.03 – 1.82	Depositor EDS
% Data completeness (in resolution range)	93.8 (44.03-1.90) 83.1 (44.03-1.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.227 , 0.243 0.237 , 0.254	Depositor DCC
R_{free} test set	1897 reflections (1.62%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.5	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 131343 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12111	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.09 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3413e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EPE, NAG, 3ZM

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	0.20	0/2709	0.37	0/3678
1	B	0.20	0/2672	0.37	0/3627
1	C	0.21	0/2709	0.38	0/3678
1	D	0.20	0/2709	0.37	0/3678
All	All	0.20	0/10799	0.37	0/14661

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	2654	0	2591	74	0
1	B	2617	0	2556	56	0
1	C	2654	0	2589	58	0
1	D	2654	0	2589	58	0
2	A	126	0	117	2	0
2	B	126	0	117	1	0
2	C	154	0	143	8	0
2	D	154	0	143	9	0
3	A	30	25	25	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	25	25	1	0
3	C	30	25	25	0	0
3	D	30	25	25	0	0
4	A	15	0	17	4	0
4	B	15	0	17	6	0
4	C	15	0	17	2	0
4	D	15	0	17	0	0
5	A	92	0	0	3	0
5	B	126	0	0	9	0
5	C	232	0	0	12	0
5	D	242	0	0	12	0
All	All	12011	100	11013	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LYS:HB2	2:D:502:NAG:H82	1.43	0.98
1:D:480:ARG:NH2	5:D:805:HOH:O	2.05	0.88
1:C:395:CYS:SG	5:C:819:HOH:O	2.32	0.86
2:D:508:NAG:H83	2:D:508:NAG:H3	1.55	0.86
1:C:480:ARG:NH2	5:C:764:HOH:O	2.10	0.85
1:D:346:THR:HG23	1:D:359:ILE:HB	1.58	0.84
1:B:446:VAL:HG21	2:B:506:NAG:H82	1.59	0.84
1:A:437:PRO:O	5:A:653:HOH:O	1.96	0.83
1:A:390:LEU:HD11	1:A:416:LEU:HD11	1.60	0.83
1:C:354:ASN:HA	2:C:508:NAG:H81	1.61	0.82
1:A:393:ASN:HA	1:A:396:ILE:HD13	1.62	0.82
1:B:77:THR:O	5:B:629:HOH:O	1.98	0.81
1:D:83:GLU:OE2	5:D:734:HOH:O	1.99	0.81
1:C:461:ASN:ND2	5:C:806:HOH:O	2.07	0.81
2:C:507:NAG:O4	5:C:749:HOH:O	2.02	0.77
1:B:103:GLN:HB3	4:B:511:EPE:H81	1.67	0.76
1:A:274:SER:HB2	1:A:284:ILE:HD12	1.67	0.76
1:B:118:PRO:HG3	1:B:426:MET:HE3	1.67	0.75
1:A:71:THR:O	5:A:683:HOH:O	2.07	0.73
1:B:119:CYS:O	5:B:725:HOH:O	2.07	0.73
1:C:333:ILE:HD12	1:C:390:LEU:HD21	1.72	0.71
1:C:62:GLU:HB3	5:C:779:HOH:O	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:THR:HG23	1:B:359:ILE:HB	1.71	0.71
1:B:98:ASN:N	5:B:701:HOH:O	2.12	0.70
1:D:62:GLU:HG3	1:D:64:GLU:H	1.56	0.70
1:D:277:LEU:HD21	1:D:352:HIS:HB3	1.73	0.69
1:B:390:LEU:HD11	1:B:416:LEU:HD11	1.74	0.69
1:C:346:THR:HG23	1:C:359:ILE:HB	1.75	0.69
1:C:65:VAL:HG11	1:C:208:ILE:HD12	1.75	0.68
1:D:65:VAL:HG11	1:D:208:ILE:HD12	1.76	0.68
1:A:274:SER:HB2	1:A:284:ILE:CD1	2.24	0.67
1:B:274:SER:N	5:B:667:HOH:O	2.13	0.67
1:C:384:TYR:CD1	1:C:421:LYS:HD2	2.30	0.67
1:A:272:ILE:CG2	1:A:284:ILE:HD11	2.26	0.66
1:B:122:LEU:HD21	1:B:200:VAL:HB	1.77	0.66
1:A:284:ILE:CG2	1:A:454:LEU:HB2	2.26	0.66
1:C:438:PRO:O	5:C:678:HOH:O	2.14	0.66
1:B:103:GLN:HB3	4:B:511:EPE:C8	2.26	0.65
1:B:289:ASN:O	5:B:668:HOH:O	2.15	0.64
1:A:272:ILE:HG22	1:A:284:ILE:HD11	1.79	0.64
1:B:411:ASN:N	5:B:672:HOH:O	2.29	0.64
1:C:415:THR:OG1	5:C:638:HOH:O	2.14	0.64
1:B:61:HIS:CD2	2:C:504:NAG:H3	2.32	0.64
1:A:277:LEU:HD21	1:A:352:HIS:HB3	1.80	0.64
1:C:369:LEU:HD13	1:C:421:LYS:NZ	2.13	0.63
2:C:503:NAG:O4	5:C:627:HOH:O	2.15	0.63
1:A:122:LEU:CD2	1:A:200:VAL:HG22	2.29	0.63
1:D:370:GLU:HB2	5:D:709:HOH:O	1.99	0.62
1:D:373:MET:HE3	1:D:384:TYR:HB3	1.82	0.62
1:D:379:ARG:NH1	5:D:630:HOH:O	2.17	0.62
1:B:86:LEU:HB3	1:B:89:VAL:HG21	1.81	0.61
1:A:446:VAL:HG21	2:A:506:NAG:H82	1.83	0.61
1:D:290:LYS:NZ	5:D:774:HOH:O	2.32	0.61
1:A:369:LEU:HD12	1:A:421:LYS:NZ	2.16	0.60
1:D:90:THR:OG1	5:D:772:HOH:O	2.16	0.60
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.37	0.60
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.37	0.60
1:A:65:VAL:HG11	1:A:115:SER:HB3	1.84	0.59
1:A:231:LYS:NZ	1:A:267:GLU:OE1	2.26	0.59
2:D:508:NAG:C8	2:D:508:NAG:H3	2.30	0.59
1:A:390:LEU:CD1	1:A:416:LEU:HD11	2.32	0.59
1:A:460:ALA:HB1	1:A:463:THR:OG1	2.03	0.59
1:A:384:TYR:OH	1:A:424:ILE:HG23	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG21	2:A:508:NAG:H5	1.85	0.58
1:D:421:LYS:NZ	1:D:421:LYS:HB3	2.20	0.57
1:C:230:ASP:HB2	1:C:233:PHE:HB2	1.88	0.56
1:C:207:LYS:HG3	1:C:439:ILE:HG22	1.88	0.56
1:C:59:LYS:HB2	1:C:62:GLU:HG3	1.88	0.56
1:B:358:THR:OG1	1:B:465:ASN:OD1	2.24	0.56
1:C:346:THR:O	1:C:350:LYS:HG3	2.06	0.55
1:A:118:PRO:HG3	1:A:426:MET:HE3	1.88	0.55
1:D:393:ASN:HD22	1:D:396:ILE:HD12	1.72	0.55
1:A:368:ASP:OD2	3:A:510:3ZM:N26	2.36	0.55
1:A:122:LEU:HD22	1:A:200:VAL:HG22	1.88	0.54
1:A:86:LEU:HB3	1:A:89:VAL:HG21	1.88	0.54
1:B:384:TYR:OH	1:B:424:ILE:HG23	2.08	0.54
1:A:284:ILE:HG22	1:A:454:LEU:O	2.07	0.54
1:B:273:ARG:HB2	1:B:285:ILE:HB	1.90	0.54
1:C:65:VAL:HG11	1:C:115:SER:HB3	1.89	0.53
1:C:103:GLN:HB3	4:C:513:EPE:H81	1.89	0.53
1:D:448:ASN:HD22	2:D:511:NAG:H83	1.72	0.53
1:C:369:LEU:HD13	1:C:421:LYS:HZ3	1.72	0.53
1:D:118:PRO:HG3	1:D:435:TYR:CZ	2.44	0.53
1:B:382:PHE:CG	1:B:424:ILE:HD13	2.44	0.53
1:D:122:LEU:HD21	5:D:832:HOH:O	2.07	0.53
1:B:265:LEU:HD21	1:B:450:THR:HG22	1.91	0.53
1:B:112:TRP:CE3	1:B:116:LEU:HD22	2.45	0.52
2:C:505:NAG:O7	5:C:737:HOH:O	2.19	0.52
1:B:118:PRO:HG3	1:B:426:MET:CE	2.37	0.52
1:B:426:MET:SD	1:B:430:THR:OG1	2.67	0.52
1:A:44:VAL:HG12	1:A:492:GLU:HB3	1.90	0.52
1:A:273:ARG:HB2	1:A:285:ILE:HB	1.92	0.52
2:D:508:NAG:H82	2:D:508:NAG:C1	2.39	0.52
1:A:423:ILE:O	1:A:424:ILE:HD13	2.10	0.52
1:C:122:LEU:O	1:C:122:LEU:HD12	2.10	0.52
1:C:65:VAL:HB	1:C:115:SER:OG	2.09	0.52
1:C:480:ARG:NE	5:C:816:HOH:O	2.40	0.51
1:A:118:PRO:HG3	1:A:426:MET:CE	2.40	0.51
1:A:421:LYS:NZ	5:A:690:HOH:O	2.13	0.51
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.93	0.51
1:D:477:ASP:OD1	1:D:480:ARG:NH1	2.44	0.51
1:C:86:LEU:HB3	1:C:89:VAL:HG21	1.92	0.51
1:C:426:MET:HE2	1:C:433:ALA:HB2	1.92	0.51
1:C:384:TYR:CG	1:C:421:LYS:HD2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG11	1:B:115:SER:HB3	1.93	0.51
1:C:106:GLU:OE1	5:C:684:HOH:O	2.19	0.51
1:C:446:VAL:HG21	2:C:506:NAG:H82	1.93	0.51
1:D:277:LEU:CD2	1:D:352:HIS:HB3	2.41	0.50
1:B:86:LEU:HB3	1:B:89:VAL:CG2	2.42	0.50
1:A:103:GLN:HB3	4:A:511:EPE:C8	2.41	0.50
1:A:419:LYS:NZ	1:B:114:GLN:OE1	2.44	0.50
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.47	0.50
1:D:240:LYS:HD2	2:D:502:NAG:C8	2.42	0.50
1:B:423:ILE:C	1:B:424:ILE:HG13	2.32	0.50
1:A:342:LEU:HD23	1:A:396:ILE:HG12	1.93	0.50
1:A:396:ILE:N	1:A:396:ILE:HD12	2.26	0.50
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.77	0.50
1:A:65:VAL:HG11	1:A:208:ILE:HD12	1.94	0.50
1:A:52:LEU:O	4:A:511:EPE:H71	2.11	0.50
1:C:422:GLN:HB3	1:C:435:TYR:O	2.12	0.50
1:A:384:TYR:CE1	1:A:424:ILE:HD12	2.47	0.50
1:C:297:THR:OG1	1:C:444:ASN:ND2	2.38	0.49
1:D:392:ASN:HA	5:D:834:HOH:O	2.10	0.49
1:B:390:LEU:CD1	1:B:416:LEU:HD11	2.42	0.49
1:C:93:PHE:HB2	1:C:233:PHE:HZ	1.77	0.49
1:D:420:ILE:HG21	1:D:438:PRO:HG3	1.95	0.49
1:D:93:PHE:HB2	1:D:233:PHE:HZ	1.78	0.49
1:B:59:LYS:NZ	5:B:709:HOH:O	2.45	0.49
1:C:265:LEU:HD11	1:C:291:SER:OG	2.12	0.49
1:D:265:LEU:HD11	1:D:291:SER:OG	2.12	0.49
4:A:511:EPE:H51	4:A:511:EPE:O8	2.13	0.49
1:A:59:LYS:HB2	1:A:62:GLU:HG3	1.95	0.49
1:A:65:VAL:CG1	1:A:115:SER:HB3	2.43	0.48
1:D:333:ILE:HD12	1:D:390:LEU:HD21	1.94	0.48
4:B:511:EPE:H51	4:B:511:EPE:O8	2.12	0.48
1:C:391:PHE:CE1	1:C:470:PRO:HG3	2.48	0.48
1:D:230:ASP:HB2	1:D:233:PHE:HB2	1.94	0.48
1:C:392:ASN:HA	5:C:772:HOH:O	2.13	0.48
1:C:337:LYS:NZ	2:C:507:NAG:H61	2.28	0.48
1:C:115:SER:HB2	1:C:116:LEU:HD12	1.95	0.48
1:A:378:CYS:HB3	1:A:383:PHE:CD1	2.48	0.48
1:D:341:VAL:O	1:D:345:VAL:HG23	2.13	0.48
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.96	0.47
1:D:426:MET:SD	1:D:430:THR:HB	2.54	0.47
1:D:327:ARG:HD2	5:D:689:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:HB3	3:A:510:3ZM:C22	2.44	0.47
1:A:369:LEU:HD12	1:A:421:LYS:HZ3	1.79	0.47
1:A:333:ILE:HD12	1:A:333:ILE:N	2.29	0.47
1:B:456:ARG:N	5:B:693:HOH:O	2.27	0.47
1:A:286:VAL:HB	1:A:452:ILE:HB	1.97	0.47
1:D:384:TYR:OH	1:D:424:ILE:HG23	2.14	0.47
1:B:346:THR:O	1:B:350:LYS:HG3	2.16	0.46
1:B:378:CYS:HB3	1:B:383:PHE:CD1	2.50	0.46
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.97	0.46
1:D:358:THR:HB	1:D:465:ASN:OD1	2.16	0.46
1:D:422:GLN:HB3	1:D:435:TYR:O	2.15	0.46
1:C:327:ARG:NH2	1:C:422:GLN:OE1	2.43	0.46
1:D:436:ALA:HB1	1:D:437:PRO:HD2	1.98	0.46
1:D:240:LYS:CB	2:D:502:NAG:H82	2.31	0.46
1:C:420:ILE:HG21	1:C:438:PRO:HG3	1.98	0.46
1:D:361:PHE:N	1:D:393:ASN:OD1	2.42	0.46
1:B:223:TYR:CE2	1:B:490:GLN:HB2	2.51	0.46
1:A:273:ARG:O	1:A:284:ILE:HD12	2.16	0.46
1:A:230:ASP:HB2	1:A:233:PHE:HB2	1.97	0.46
1:C:65:VAL:CG1	1:C:115:SER:HB3	2.46	0.46
1:C:230:ASP:OD1	1:C:241:ASN:HB2	2.16	0.46
1:C:337:LYS:HZ3	2:C:507:NAG:H61	1.81	0.45
1:D:290:LYS:HE2	5:D:675:HOH:O	2.16	0.45
1:A:341:VAL:O	1:A:345:VAL:HG23	2.16	0.45
1:B:370:GLU:HB3	3:B:510:3ZM:C22	2.46	0.45
1:A:369:LEU:HD12	1:A:421:LYS:HZ2	1.82	0.45
1:D:270:ILE:O	1:D:348:LYS:HE2	2.16	0.45
1:B:332:GLU:C	1:B:333:ILE:HD12	2.37	0.45
1:D:419:LYS:NZ	5:D:742:HOH:O	2.49	0.45
1:B:270:ILE:O	1:B:348:LYS:HE3	2.17	0.45
1:C:436:ALA:HB1	1:C:437:PRO:HD2	1.99	0.44
1:C:341:VAL:O	1:C:345:VAL:HG23	2.17	0.44
1:D:78:ASP:O	1:D:81:PRO:HD3	2.17	0.44
1:B:341:VAL:O	1:B:345:VAL:HG23	2.16	0.44
1:C:116:LEU:N	1:C:116:LEU:HD12	2.32	0.44
1:D:53:PHE:CZ	1:D:218:CYS:HB2	2.52	0.44
1:A:112:TRP:CD2	1:A:116:LEU:HD12	2.53	0.44
1:A:198:GLY:O	1:C:90:THR:HG21	2.17	0.44
1:A:116:LEU:CD2	1:A:208:ILE:HD11	2.48	0.44
1:B:65:VAL:HG11	1:B:208:ILE:HD12	2.00	0.44
1:B:52:LEU:O	4:B:511:EPE:H71	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:CYS:HA	1:C:331:CYS:HA	2.00	0.44
1:A:420:ILE:HG21	1:A:438:PRO:HG3	1.98	0.44
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.53	0.44
1:D:369:LEU:HD22	1:D:373:MET:HE2	2.00	0.43
1:A:59:LYS:N	1:A:59:LYS:HD2	2.33	0.43
1:C:231:LYS:HG2	1:C:267:GLU:OE1	2.17	0.43
1:D:116:LEU:HD12	1:D:116:LEU:N	2.32	0.43
1:C:273:ARG:HB2	1:C:285:ILE:HB	2.01	0.43
1:D:273:ARG:HB2	1:D:285:ILE:HB	2.01	0.43
1:D:231:LYS:HG2	1:D:267:GLU:OE1	2.18	0.43
1:A:278:THR:O	1:A:456:ARG:NH2	2.51	0.43
1:A:123:THR:HB	1:A:430:THR:O	2.19	0.43
1:A:422:GLN:HB3	1:A:435:TYR:O	2.19	0.43
1:D:118:PRO:HG3	1:D:435:TYR:CE2	2.54	0.43
1:C:348:LYS:HA	1:C:348:LYS:HD2	1.85	0.43
1:B:386:ASN:OD1	1:B:388:THR:HG23	2.19	0.43
1:B:91:GLU:HG3	1:B:226:LEU:HD13	2.01	0.43
1:A:369:LEU:HA	1:A:372:THR:OG1	2.19	0.43
1:B:52:LEU:CD2	1:B:219:THR:HG22	2.49	0.43
1:D:121:LYS:HG3	1:D:201:ILE:HB	2.01	0.43
1:B:123:THR:HB	1:B:430:THR:O	2.19	0.42
1:A:265:LEU:HD11	1:A:291:SER:OG	2.18	0.42
2:D:508:NAG:C8	2:D:508:NAG:C1	2.97	0.42
1:A:86:LEU:HB3	1:A:89:VAL:CG2	2.49	0.42
1:C:103:GLN:HB3	4:C:513:EPE:C8	2.49	0.42
1:A:257:THR:O	1:A:259:LEU:N	2.47	0.42
1:B:231:LYS:NZ	1:B:267:GLU:OE1	2.48	0.42
1:B:107:ASP:OD1	4:B:511:EPE:H52	2.19	0.42
1:D:370:GLU:OE1	5:D:709:HOH:O	2.22	0.42
1:D:255:VAL:HG13	1:D:475:ILE:HD12	2.00	0.42
1:A:370:GLU:HG2	3:A:510:3ZM:C14	2.49	0.42
1:B:231:LYS:HD3	1:B:268:GLU:OE2	2.19	0.42
1:B:257:THR:O	1:B:259:LEU:N	2.49	0.42
1:A:102:GLU:O	1:A:106:GLU:HG3	2.19	0.42
1:C:116:LEU:HD11	1:C:210:PHE:CE2	2.55	0.42
1:A:103:GLN:HB3	4:A:511:EPE:O8	2.20	0.42
1:D:384:TYR:OH	1:D:424:ILE:HD12	2.19	0.42
1:B:102:GLU:O	1:B:106:GLU:HG3	2.20	0.42
1:C:298:ARG:NH2	1:C:439:ILE:O	2.53	0.41
1:A:346:THR:HG23	1:A:359:ILE:HB	2.01	0.41
1:A:350:LYS:HG2	1:A:359:ILE:HG12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:GLU:OE1	1:D:66:HIS:HB2	2.21	0.41
1:A:222:GLY:O	1:A:491:ILE:HG12	2.20	0.41
1:B:106:GLU:OE1	5:B:666:HOH:O	2.21	0.41
1:C:53:PHE:CZ	1:C:218:CYS:HB2	2.56	0.41
1:D:421:LYS:HB2	1:D:424:ILE:HD11	2.03	0.41
1:D:384:TYR:CE1	1:D:424:ILE:HD12	2.55	0.41
1:B:333:ILE:HD12	1:B:333:ILE:N	2.36	0.41
1:A:219:THR:HG23	1:A:225:ILE:CG1	2.51	0.41
1:B:437:PRO:HA	1:B:438:PRO:HD3	1.91	0.41
1:D:86:LEU:HB3	1:D:89:VAL:HG21	2.03	0.41
1:D:240:LYS:HD2	2:D:502:NAG:H83	2.01	0.41
1:C:101:VAL:HG21	1:C:480:ARG:HG2	2.02	0.41
1:A:421:LYS:HG2	4:B:511:EPE:O2S	2.21	0.41
1:C:64:GLU:OE1	1:C:66:HIS:HB2	2.21	0.41
1:C:381:GLU:HG3	1:C:443:ILE:HD13	2.03	0.41
1:B:78:ASP:HA	1:B:79:PRO:HD3	1.97	0.41
1:D:423:ILE:O	1:D:424:ILE:HD13	2.21	0.40
1:C:361:PHE:O	1:C:393:ASN:ND2	2.36	0.40
1:A:56:SER:C	1:A:77:THR:HG23	2.42	0.40
1:C:363:PRO:O	1:C:469:ARG:NH1	2.40	0.40
1:D:117:GLN:HA	1:D:118:PRO:HD3	1.87	0.40
1:A:111:LEU:HD23	1:A:111:LEU:C	2.41	0.40
1:D:122:LEU:HD12	1:D:122:LEU:O	2.21	0.40
1:B:59:LYS:HD2	1:B:59:LYS:N	2.36	0.40
1:B:369:LEU:HA	1:B:372:THR:OG1	2.22	0.40
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.56	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	333/353 (94%)	319 (96%)	14 (4%)	0	100	100
1	B	328/353 (93%)	316 (96%)	12 (4%)	0	100	100
1	C	333/353 (94%)	320 (96%)	12 (4%)	1 (0%)	46	35
1	D	333/353 (94%)	322 (97%)	11 (3%)	0	100	100
All	All	1327/1412 (94%)	1277 (96%)	49 (4%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	GLY

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	303/311 (97%)	303 (100%)	0	100	100
1	B	298/311 (96%)	298 (100%)	0	100	100
1	C	303/311 (97%)	303 (100%)	0	100	100
1	D	303/311 (97%)	303 (100%)	0	100	100
All	All	1207/1244 (97%)	1207 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

48 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	501	1	14,14,15	0.20	0	15,19,21	0.26	0
2	NAG	A	502	1	14,14,15	0.23	0	15,19,21	0.32	0
2	NAG	A	503	1	14,14,15	0.21	0	15,19,21	0.45	0
2	NAG	A	504	1	14,14,15	0.22	0	15,19,21	0.34	0
2	NAG	A	505	1	14,14,15	0.23	0	15,19,21	0.33	0
2	NAG	A	506	1	14,14,15	0.22	0	15,19,21	0.38	0
2	NAG	A	507	1	14,14,15	0.28	0	15,19,21	0.39	0
2	NAG	A	508	1	14,14,15	0.23	0	15,19,21	0.32	0
2	NAG	A	509	1	14,14,15	0.21	0	15,19,21	0.33	0
3	3ZM	A	510	-	31,33,33	3.12	10 (32%)	25,46,46	2.75	11 (44%)
4	EPE	A	511	-	15,15,15	0.79	1 (6%)	19,20,20	1.94	6 (31%)
2	NAG	B	501	1	14,14,15	0.21	0	15,19,21	0.26	0
2	NAG	B	502	1	14,14,15	0.23	0	15,19,21	0.34	0
2	NAG	B	503	1	14,14,15	0.20	0	15,19,21	0.48	0
2	NAG	B	504	1	14,14,15	0.23	0	15,19,21	0.33	0
2	NAG	B	505	1	14,14,15	0.21	0	15,19,21	0.33	0
2	NAG	B	506	1	14,14,15	0.25	0	15,19,21	0.36	0
2	NAG	B	507	1	14,14,15	0.35	0	15,19,21	0.46	0
2	NAG	B	508	1	14,14,15	0.23	0	15,19,21	0.36	0
2	NAG	B	509	1	14,14,15	0.21	0	15,19,21	0.32	0
3	3ZM	B	510	-	31,33,33	3.09	10 (32%)	25,46,46	2.75	11 (44%)
4	EPE	B	511	-	15,15,15	0.79	1 (6%)	19,20,20	2.13	6 (31%)
2	NAG	C	501	1	14,14,15	0.19	0	15,19,21	0.27	0
2	NAG	C	502	1	14,14,15	0.24	0	15,19,21	0.41	0
2	NAG	C	503	1	14,14,15	0.29	0	15,19,21	0.39	0
2	NAG	C	504	1	14,14,15	0.29	0	15,19,21	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	505	1	14,14,15	0.25	0	15,19,21	0.38	0
2	NAG	C	506	1	14,14,15	0.24	0	15,19,21	0.35	0
2	NAG	C	507	1	14,14,15	0.32	0	15,19,21	0.44	0
2	NAG	C	508	1	14,14,15	0.29	0	15,19,21	0.38	0
2	NAG	C	509	1	14,14,15	0.24	0	15,19,21	0.35	0
2	NAG	C	510	1	14,14,15	0.25	0	15,19,21	0.38	0
2	NAG	C	511	1	14,14,15	0.21	0	15,19,21	0.38	0
3	3ZM	C	512	-	31,33,33	2.98	10 (32%)	25,46,46	2.62	10 (40%)
4	EPE	C	513	-	15,15,15	0.81	1 (6%)	19,20,20	1.98	6 (31%)
2	NAG	D	501	1	14,14,15	0.21	0	15,19,21	0.25	0
2	NAG	D	502	1	14,14,15	0.22	0	15,19,21	0.36	0
2	NAG	D	503	1	14,14,15	0.27	0	15,19,21	0.41	0
2	NAG	D	504	1	14,14,15	0.25	0	15,19,21	0.31	0
2	NAG	D	505	1	14,14,15	0.25	0	15,19,21	0.36	0
2	NAG	D	506	1	14,14,15	0.24	0	15,19,21	0.34	0
2	NAG	D	507	1	14,14,15	0.27	0	15,19,21	0.39	0
2	NAG	D	508	1	14,14,15	0.27	0	15,19,21	0.43	0
2	NAG	D	509	1	14,14,15	0.24	0	15,19,21	0.35	0
2	NAG	D	510	1	14,14,15	0.24	0	15,19,21	0.40	0
2	NAG	D	511	1	14,14,15	0.21	0	15,19,21	0.35	0
3	3ZM	D	512	-	31,33,33	2.97	10 (32%)	25,46,46	2.66	10 (40%)
4	EPE	D	513	-	15,15,15	0.79	1 (6%)	19,20,20	2.11	7 (36%)

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	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	0/6/23/26	0/1/1/1
3	3ZM	A	510	-	-	0/12/30/30	0/4/4/4
4	EPE	A	511	-	-	0/9/19/19	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1	-	0/6/23/26	0/1/1/1
3	3ZM	B	510	-	-	0/12/30/30	0/4/4/4
4	EPE	B	511	-	-	0/9/19/19	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	503	1	-	0/6/23/26	0/1/1/1
2	NAG	C	504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	505	1	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1	-	0/6/23/26	0/1/1/1
2	NAG	C	507	1	-	0/6/23/26	0/1/1/1
2	NAG	C	508	1	-	0/6/23/26	0/1/1/1
2	NAG	C	509	1	-	0/6/23/26	0/1/1/1
2	NAG	C	510	1	-	0/6/23/26	0/1/1/1
2	NAG	C	511	1	-	0/6/23/26	0/1/1/1
3	3ZM	C	512	-	-	0/12/30/30	0/4/4/4
4	EPE	C	513	-	-	0/9/19/19	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
2	NAG	D	503	1	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1	-	0/6/23/26	0/1/1/1
2	NAG	D	505	1	-	0/6/23/26	0/1/1/1
2	NAG	D	506	1	-	0/6/23/26	0/1/1/1
2	NAG	D	507	1	-	0/6/23/26	0/1/1/1
2	NAG	D	508	1	-	0/6/23/26	0/1/1/1
2	NAG	D	509	1	-	0/6/23/26	0/1/1/1
2	NAG	D	510	1	-	0/6/23/26	0/1/1/1
2	NAG	D	511	1	-	0/6/23/26	0/1/1/1
3	3ZM	D	512	-	-	0/12/30/30	0/4/4/4
4	EPE	D	513	-	-	0/9/19/19	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	510	3ZM	C05-C03	-2.30	1.38	1.42
3	C	512	3ZM	C05-C03	-2.29	1.38	1.42
3	D	512	3ZM	C05-C03	-2.25	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	510	3ZM	C05-C03	-2.20	1.38	1.42
3	C	512	3ZM	C18-CL21	2.26	1.79	1.74
3	D	512	3ZM	C18-CL21	2.35	1.79	1.74
3	C	512	3ZM	C25-N26	2.50	1.50	1.47
3	D	512	3ZM	C25-N26	2.58	1.50	1.47
3	B	510	3ZM	C25-N26	2.59	1.50	1.47
3	A	510	3ZM	C25-N26	2.64	1.50	1.47
4	B	511	EPE	C10-S	2.64	1.81	1.77
4	A	511	EPE	C10-S	2.65	1.81	1.77
4	C	513	EPE	C10-S	2.67	1.81	1.77
3	B	510	3ZM	C18-CL21	2.68	1.80	1.74
4	D	513	EPE	C10-S	2.69	1.81	1.77
3	A	510	3ZM	C18-CL21	2.79	1.80	1.74
3	C	512	3ZM	C11-N10	4.24	1.43	1.34
3	C	512	3ZM	C12-N13	4.26	1.43	1.36
3	C	512	3ZM	C09-N10	4.32	1.54	1.46
3	B	510	3ZM	C11-N10	4.45	1.44	1.34
3	D	512	3ZM	C11-N10	4.46	1.44	1.34
3	A	510	3ZM	C11-N10	4.51	1.44	1.34
3	B	510	3ZM	C12-N13	4.57	1.43	1.36
3	C	512	3ZM	C14-N13	4.63	1.44	1.36
3	D	512	3ZM	C12-N13	4.65	1.44	1.36
3	A	510	3ZM	C12-N13	4.80	1.44	1.36
3	D	512	3ZM	C14-N13	4.84	1.44	1.36
3	B	510	3ZM	C14-N13	4.85	1.44	1.36
3	A	510	3ZM	C09-N10	4.89	1.55	1.46
3	B	510	3ZM	C09-N10	4.90	1.55	1.46
3	D	512	3ZM	C09-N10	4.91	1.55	1.46
3	A	510	3ZM	C14-N13	5.09	1.44	1.36
3	D	512	3ZM	C09-C25	6.34	1.64	1.54
3	A	510	3ZM	C09-C25	6.49	1.64	1.54
3	B	510	3ZM	C09-C25	6.53	1.64	1.54
3	C	512	3ZM	C09-C25	6.94	1.64	1.54
3	C	512	3ZM	C15-C14	7.13	1.57	1.47
3	D	512	3ZM	C15-C14	7.20	1.57	1.47
3	D	512	3ZM	C01-C09	7.47	1.59	1.51
3	A	510	3ZM	C01-C09	7.74	1.59	1.51
3	B	510	3ZM	C01-C09	7.81	1.59	1.51
3	B	510	3ZM	C15-C14	8.02	1.59	1.47
3	C	512	3ZM	C01-C09	8.14	1.59	1.51
3	A	510	3ZM	C15-C14	8.16	1.59	1.47

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	510	3ZM	O24-C11-N10	-4.12	114.99	122.45
3	A	510	3ZM	O24-C11-N10	-3.99	115.23	122.45
3	C	512	3ZM	O24-C11-N10	-3.49	116.14	122.45
3	D	512	3ZM	O24-C11-N10	-3.35	116.39	122.45
3	A	510	3ZM	C16-C15-C20	-3.06	111.58	117.56
3	B	510	3ZM	C16-C15-C20	-3.03	111.64	117.56
3	D	512	3ZM	C16-C15-C20	-2.98	111.75	117.56
3	C	512	3ZM	C16-C15-C20	-2.94	111.82	117.56
4	D	513	EPE	C5-C6-N1	-2.19	106.39	110.65
3	B	510	3ZM	C17-C16-C15	2.00	123.96	121.15
4	D	513	EPE	O3S-S-C10	2.01	109.16	104.99
3	B	510	3ZM	C22-C23-C12	2.01	108.92	107.59
3	D	512	3ZM	C22-C23-C12	2.10	108.98	107.59
3	A	510	3ZM	C17-C16-C15	2.10	124.10	121.15
4	B	511	EPE	O3S-S-C10	2.10	109.36	104.99
3	C	512	3ZM	C29-C30-C25	2.11	114.34	111.45
4	A	511	EPE	O3S-S-C10	2.11	109.38	104.99
3	A	510	3ZM	C22-C23-C12	2.19	109.04	107.59
4	C	513	EPE	O3S-S-C10	2.20	109.56	104.99
3	C	512	3ZM	C01-C09-C25	2.39	114.94	111.00
3	D	512	3ZM	C29-C30-C25	2.56	114.95	111.45
4	D	513	EPE	C7-N4-C3	2.61	116.92	111.25
3	B	510	3ZM	C09-N10-C11	2.62	126.37	121.97
3	A	510	3ZM	C29-C30-C25	2.73	115.20	111.45
3	B	510	3ZM	C29-C30-C25	2.75	115.22	111.45
4	D	513	EPE	C7-N4-C5	2.86	117.48	111.25
3	A	510	3ZM	C09-N10-C11	2.91	126.85	121.97
4	C	513	EPE	C5-N4-C3	3.00	115.59	108.87
4	A	511	EPE	C7-N4-C3	3.13	118.06	111.25
4	C	513	EPE	O2S-S-C10	3.28	109.19	106.87
4	A	511	EPE	O2S-S-C10	3.32	109.22	106.87
4	D	513	EPE	O2S-S-C10	3.35	109.24	106.87
4	B	511	EPE	O2S-S-C10	3.37	109.25	106.87
3	C	512	3ZM	C09-N10-C11	3.41	127.69	121.97
3	A	510	3ZM	C19-C20-C15	3.41	125.94	121.15
4	C	513	EPE	C7-N4-C3	3.43	118.71	111.25
3	B	510	3ZM	C19-C20-C15	3.43	125.97	121.15
3	C	512	3ZM	C19-C20-C15	3.44	125.98	121.15
3	D	512	3ZM	C19-C20-C15	3.44	125.99	121.15
4	B	511	EPE	C7-N4-C3	3.57	119.02	111.25
4	A	511	EPE	C5-N4-C3	3.59	116.90	108.87
3	C	512	3ZM	C20-C15-C14	3.60	126.75	120.68
4	A	511	EPE	C7-N4-C5	3.61	119.10	111.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	512	3ZM	C20-C15-C14	3.71	126.93	120.68
3	D	512	3ZM	C09-N10-C11	3.72	128.21	121.97
4	A	511	EPE	O1S-S-C10	3.72	109.50	106.87
3	C	512	3ZM	C27-N26-C25	3.74	114.07	111.58
4	C	513	EPE	O1S-S-C10	3.75	109.52	106.87
3	B	510	3ZM	C20-C15-C14	3.84	127.15	120.68
4	B	511	EPE	O1S-S-C10	3.89	109.62	106.87
4	C	513	EPE	C7-N4-C5	3.97	119.90	111.25
3	D	512	3ZM	C27-N26-C25	4.08	114.30	111.58
4	D	513	EPE	O1S-S-C10	4.14	109.79	106.87
3	A	510	3ZM	C20-C15-C14	4.14	127.66	120.68
4	B	511	EPE	C7-N4-C5	4.18	120.34	111.25
3	A	510	3ZM	C27-N26-C25	4.21	114.39	111.58
4	B	511	EPE	C5-N4-C3	4.25	118.38	108.87
3	C	512	3ZM	C23-C22-C14	4.46	110.54	107.59
3	D	512	3ZM	C23-C22-C14	4.49	110.57	107.59
4	D	513	EPE	C5-N4-C3	4.69	119.36	108.87
3	B	510	3ZM	C23-C22-C14	4.72	110.71	107.59
3	B	510	3ZM	C27-N26-C25	4.73	114.74	111.58
3	A	510	3ZM	C23-C22-C14	4.92	110.85	107.59
3	D	512	3ZM	C07-C05-C03	7.66	136.69	127.36
3	C	512	3ZM	C07-C05-C03	7.68	136.72	127.36
3	A	510	3ZM	C07-C05-C03	7.71	136.75	127.36
3	B	510	3ZM	C07-C05-C03	7.73	136.78	127.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	506	NAG	1	0
2	A	508	NAG	1	0
3	A	510	3ZM	3	0
4	A	511	EPE	4	0
2	B	506	NAG	1	0
3	B	510	3ZM	1	0
4	B	511	EPE	6	0
2	C	503	NAG	1	0
2	C	504	NAG	1	0
2	C	505	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	506	NAG	1	0
2	C	507	NAG	3	0
2	C	508	NAG	1	0
4	C	513	EPE	2	0
2	D	502	NAG	4	0
2	D	508	NAG	4	0
2	D	511	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	339/353 (96%)	1.14	62 (18%) 2 2	36, 69, 117, 167	0
1	B	334/353 (94%)	0.98	50 (14%) 3 3	33, 63, 101, 134	0
1	C	339/353 (96%)	0.39	13 (3%) 44 48	27, 44, 78, 127	0
1	D	339/353 (96%)	0.39	14 (4%) 41 45	27, 43, 77, 112	0
All	All	1351/1412 (95%)	0.73	139 (10%) 9 9	27, 53, 101, 167	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	THR	13.3
1	D	324	GLY	11.0
1	D	123	THR	10.0
1	D	124	GLY	9.5
1	C	122	LEU	9.3
1	A	44	VAL	9.1
1	D	122	LEU	9.1
1	A	301	ASN	9.0
1	A	461	ASN	8.4
1	B	123	THR	8.4
1	C	198	GLY	8.3
1	A	462	ASN	7.4
1	B	459	GLY	7.3
1	D	198	GLY	6.8
1	B	365	SER	6.8
1	B	124	GLY	6.8
1	A	458	GLY	6.4
1	A	123	THR	6.3
1	C	324	GLY	6.1
1	A	354	ASN	6.1
1	B	301	ASN	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	199	SER	5.9
1	A	324	GLY	5.9
1	B	460	ALA	5.8
1	A	358	THR	5.8
1	A	465	ASN	5.6
1	B	44	VAL	5.5
1	B	465	ASN	5.5
1	C	124	GLY	5.5
1	A	353	PHE	5.4
1	B	463	THR	5.4
1	C	199	SER	5.4
1	C	301	ASN	5.4
1	D	301	ASN	5.4
1	A	492	GLU	5.2
1	D	492	GLU	5.1
1	A	198	GLY	5.0
1	A	365	SER	5.0
1	A	392	ASN	5.0
1	B	458	GLY	4.9
1	B	492	GLU	4.9
1	B	200	VAL	4.8
1	A	82	GLN	4.8
1	B	82	GLN	4.8
1	A	325	ASP	4.7
1	B	89	VAL	4.7
1	B	464	SER	4.6
1	B	353	PHE	4.6
1	B	324	GLY	4.6
1	B	491	ILE	4.4
1	B	326	ILE	4.3
1	A	391	PHE	4.2
1	B	462	ASN	4.2
1	A	393	ASN	4.2
1	A	360	ILE	4.2
1	B	84	ILE	4.2
1	A	396	ILE	4.1
1	A	277	LEU	4.1
1	A	395	CYS	4.1
1	B	45	TRP	4.0
1	B	199	SER	4.0
1	A	89	VAL	3.9
1	A	491	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	201	ILE	3.9
1	B	357	LYS	3.9
1	B	461	ASN	3.8
1	A	201	ILE	3.8
1	A	122	LEU	3.7
1	A	84	ILE	3.7
1	A	350	LYS	3.7
1	B	411	ASN	3.6
1	B	358	THR	3.6
1	B	354	ASN	3.5
1	D	44	VAL	3.5
1	A	352	HIS	3.5
1	A	414	ILE	3.4
1	A	199	SER	3.4
1	D	365	SER	3.3
1	A	359	ILE	3.3
1	B	86	LEU	3.3
1	C	440	ASP	3.3
1	A	411	ASN	3.2
1	A	357	LYS	3.2
1	D	395	CYS	3.2
1	B	272	ILE	3.2
1	A	362	GLN	3.2
1	D	201	ILE	3.2
1	B	281	ALA	3.1
1	B	276	ASN	3.1
1	B	122	LEU	3.1
1	B	359	ILE	3.1
1	A	224	VAL	3.0
1	A	467	THR	3.0
1	C	200	VAL	3.0
1	A	394	THR	3.0
1	A	87	GLU	3.0
1	A	200	VAL	2.9
1	A	45	TRP	2.9
1	A	463	THR	2.9
1	A	85	HIS	2.9
1	A	366	GLY	2.9
1	B	350	LYS	2.8
1	A	355	ASN	2.7
1	A	124	GLY	2.7
1	A	272	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	492	GLU	2.7
1	D	277	LEU	2.6
1	A	46	LYS	2.6
1	C	421	LYS	2.6
1	A	276	ASN	2.6
1	B	424	ILE	2.6
1	B	80	ASN	2.5
1	B	277	LEU	2.4
1	A	351	GLU	2.4
1	B	278	THR	2.4
1	A	412	GLY	2.4
1	D	424	ILE	2.4
1	B	62	GLU	2.3
1	B	93	PHE	2.3
1	A	464	SER	2.3
1	B	355	ASN	2.3
1	B	46	LYS	2.3
1	B	202	LYS	2.2
1	B	343	LYS	2.2
1	A	369	LEU	2.2
1	A	235	GLY	2.2
1	A	459	GLY	2.2
1	B	360	ILE	2.2
1	C	441	GLY	2.2
1	B	201	ILE	2.2
1	B	69	TRP	2.2
1	A	424	ILE	2.1
1	A	278	THR	2.1
1	A	281	ALA	2.1
1	A	346	THR	2.1
1	A	343	LYS	2.1
1	A	80	ASN	2.1
1	B	349	LEU	2.1
1	B	414	ILE	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
2	NAG	C	511	14/15	0.63	0.29	8.54	71,85,90,93	0
2	NAG	D	511	14/15	0.68	0.30	6.88	71,83,87,90	0
3	3ZM	A	510	30/30	0.68	0.34	6.58	61,119,148,152	0
2	NAG	B	508	14/15	0.70	0.29	6.54	70,80,83,85	0
2	NAG	A	506	14/15	0.79	0.22	5.41	49,62,74,78	0
3	3ZM	B	510	30/30	0.74	0.28	4.15	46,110,134,137	0
3	3ZM	D	512	30/30	0.77	0.24	2.74	48,87,111,111	0
2	NAG	A	505	14/15	0.73	0.24	2.72	71,80,87,87	0
2	NAG	B	507	14/15	0.79	0.36	2.52	71,83,91,95	0
2	NAG	B	501	14/15	0.87	0.30	2.47	63,75,78,78	0
2	NAG	C	507	14/15	0.84	0.18	2.21	44,52,61,67	0
2	NAG	D	506	14/15	0.87	0.16	2.00	47,58,63,63	0
3	3ZM	C	512	30/30	0.85	0.19	1.88	43,73,95,95	0
2	NAG	A	508	14/15	0.74	0.25	1.58	60,71,75,75	0
2	NAG	C	506	14/15	0.80	0.26	1.45	54,67,73,74	0
2	NAG	A	501	14/15	0.90	0.28	1.24	67,76,79,79	0
4	EPE	A	511	15/15	0.93	0.17	1.21	63,67,80,83	0
2	NAG	C	501	14/15	0.87	0.12	1.17	50,63,66,68	0
2	NAG	B	505	14/15	0.83	0.20	1.04	56,66,70,71	0
2	NAG	B	506	14/15	0.82	0.14	0.94	49,62,71,73	0
2	NAG	D	507	14/15	0.88	0.15	0.92	44,53,61,67	0
4	EPE	B	511	15/15	0.93	0.16	0.78	62,66,70,71	0
2	NAG	C	508	14/15	0.88	0.13	0.57	35,40,54,63	0
2	NAG	A	509	14/15	0.81	0.16	0.56	53,61,64,66	0
4	EPE	D	513	15/15	0.96	0.16	0.55	33,39,50,50	0
2	NAG	D	501	14/15	0.91	0.12	0.02	49,62,65,66	0
2	NAG	D	505	14/15	0.89	0.12	0.02	40,49,57,61	0
4	EPE	C	513	15/15	0.97	0.13	-0.02	39,42,46,53	0
2	NAG	D	508	14/15	0.91	0.13	-0.07	40,46,67,68	0
2	NAG	B	503	14/15	0.95	0.12	-0.24	29,34,36,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	D	503	14/15	0.94	0.14	-0.25	29,35,41,41	0
2	NAG	C	505	14/15	0.91	0.11	-0.95	40,50,56,60	0
2	NAG	A	503	14/15	0.94	0.11	-0.97	29,33,39,39	0
2	NAG	B	509	14/15	0.91	0.12	-1.14	47,57,63,67	0
2	NAG	C	503	14/15	0.91	0.11	-1.58	30,35,42,46	0
2	NAG	A	502	14/15	0.92	0.23	-	76,87,90,92	0
2	NAG	D	509	14/15	0.92	0.11	-	45,55,60,66	0
2	NAG	A	507	14/15	0.74	0.32	-	73,84,88,88	0
2	NAG	D	504	14/15	0.92	0.10	-	43,53,60,64	0
2	NAG	B	504	14/15	0.64	0.38	-	69,77,81,83	0
2	NAG	C	502	14/15	0.36	0.47	-	93,101,106,108	0
2	NAG	D	510	14/15	0.73	0.33	-	92,96,100,101	0
2	NAG	A	504	14/15	0.55	0.42	-	75,84,86,89	0
2	NAG	D	502	14/15	0.75	0.49	-	82,92,97,98	0
2	NAG	C	504	14/15	0.77	0.15	-	43,57,62,64	0
2	NAG	B	502	14/15	0.89	0.21	-	69,81,88,90	0
2	NAG	C	509	14/15	0.92	0.11	-	42,53,58,59	0
2	NAG	C	510	14/15	0.75	0.28	-	84,91,94,97	0

6.5 Other polymers (i)

There are no such residues in this entry.