Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:50 AM GMT

PDB ID	:	3CCB
Title	:	Crystal Structure of Human DPP4 in complex with a benzimidazole derivative
Authors	:	Wallace, M.B.; Skene, R.J.
Deposited on	:	2008-02-25
Resolution	:	2.49 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:

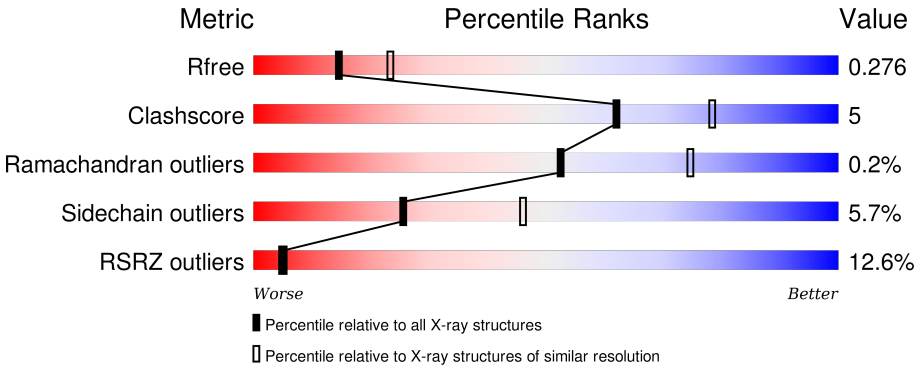
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	740	12% 81% 15%
1	B	740	6% 83% 13%
1	C	740	13% 83% 14%
1	D	740	18% 81% 15%

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	808	-	-	-	X
2	NAG	C	802	-	-	-	X
2	NAG	D	804	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24805 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	1	0
			5935	3812	977	1120	26			
1	B	729	Total	C	N	O	S	0	0	0
			5965	3830	983	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5936	3813	977	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

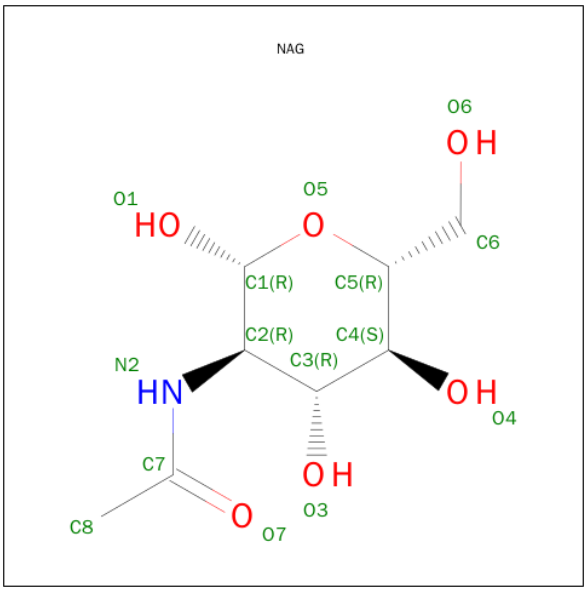
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487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

Continued on next page...

Continued from previous page...

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

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

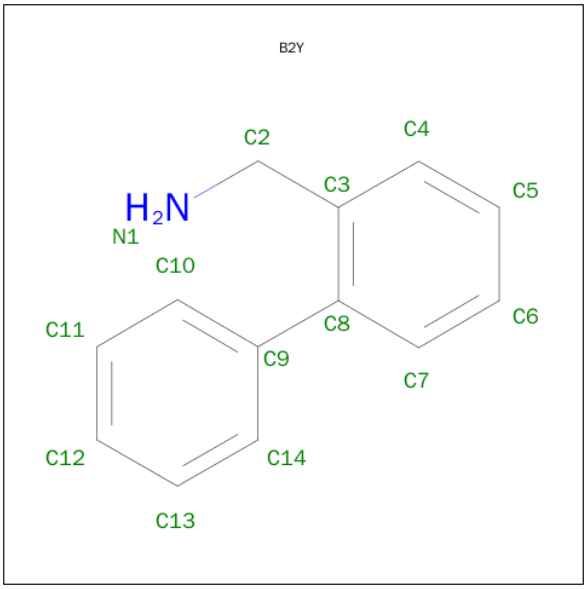


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total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

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

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

- Molecule 4 is 1-BIPHENYL-2-YLMETHANAMINE (three-letter code: B2Y) (formula: $C_{13}H_{13}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 14 13 1	0	0
4	B	1	Total C N 14 13 1	0	0
4	C	1	Total C N 14 13 1	0	0
4	D	1	Total C N 14 13 1	0	0

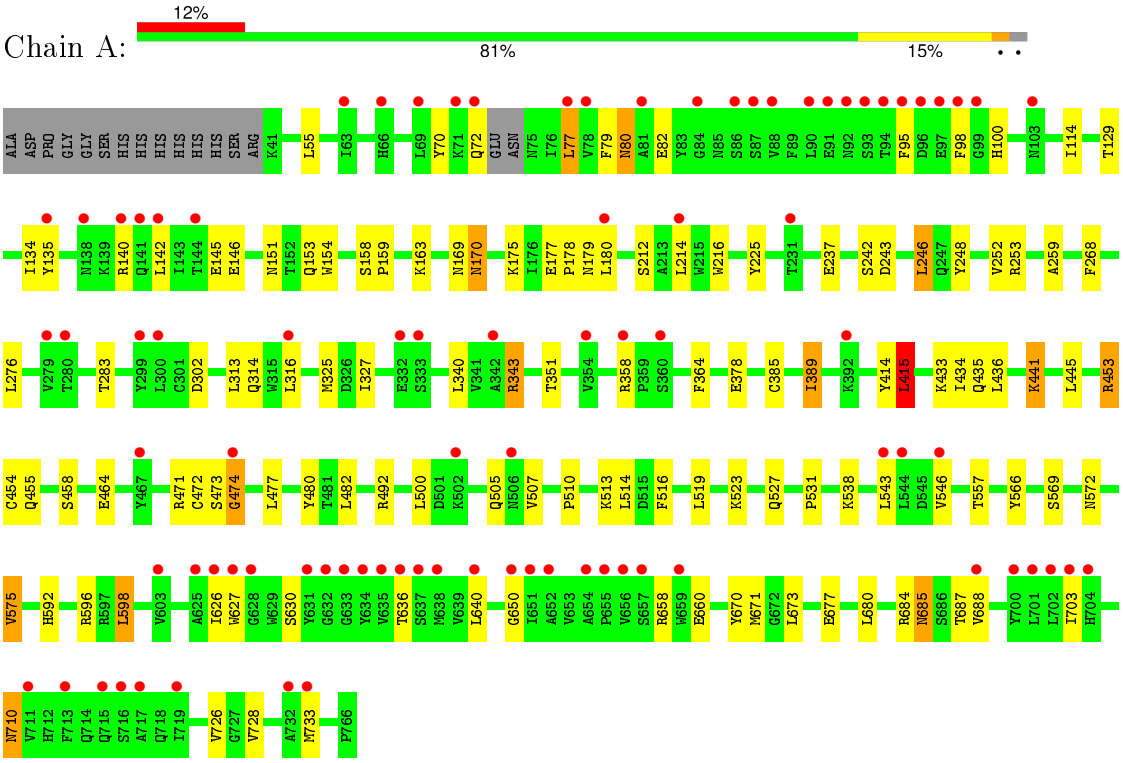
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	206	Total O 206 206	0	0
5	B	191	Total O 191 191	0	0
5	C	189	Total O 189 189	0	0
5	D	90	Total O 90 90	0	0

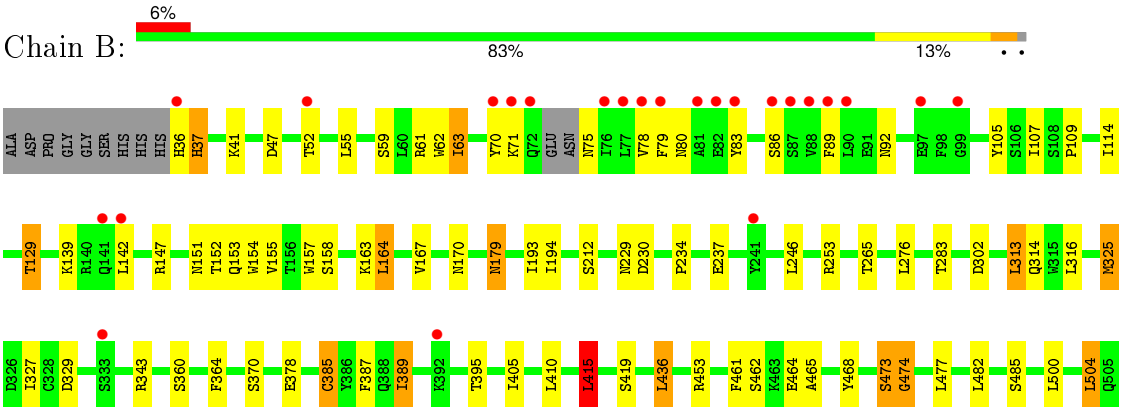
3 Residue-property plots (i)

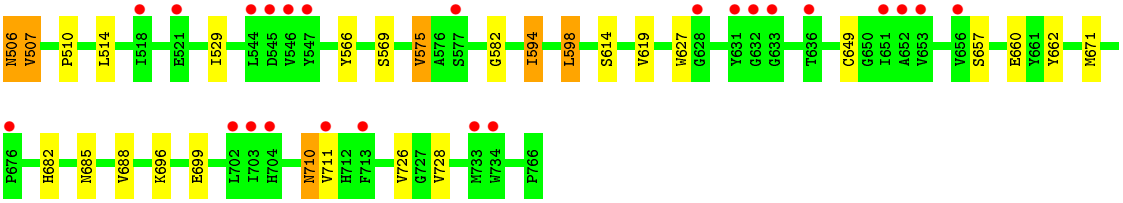
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Dipeptidyl peptidase 4



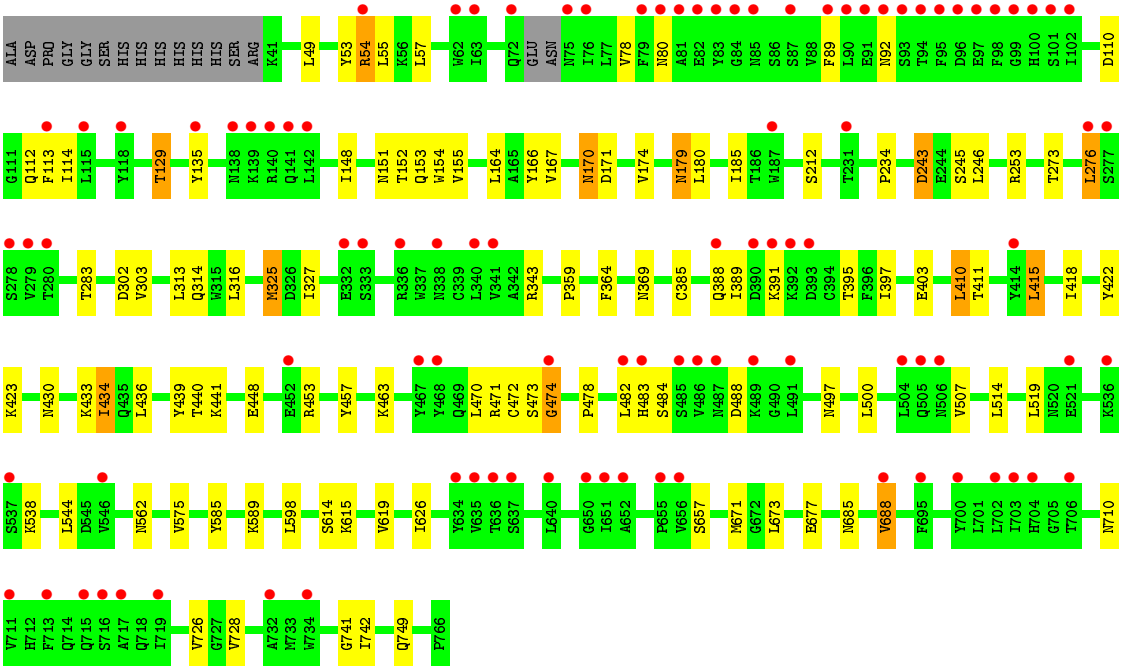
- Molecule 1: Dipeptidyl peptidase 4





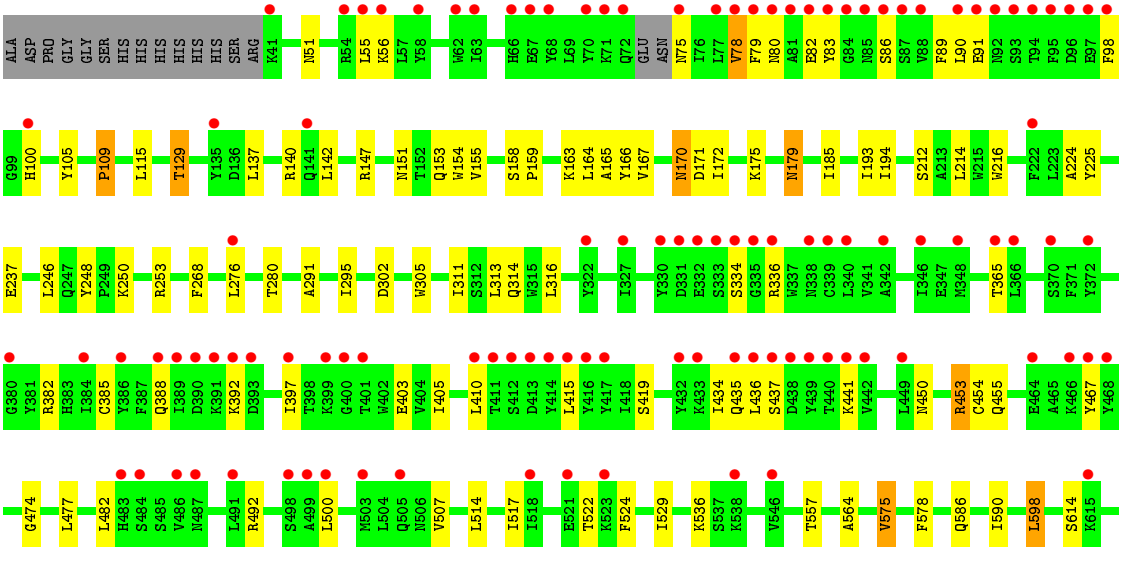
• Molecule 1: Dipeptidyl peptidase 4

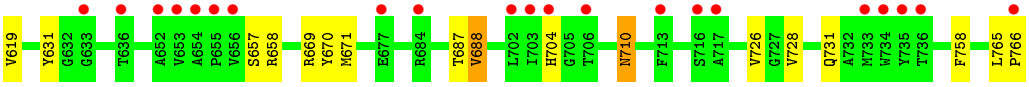
Chain C:



• Molecule 1: Dipeptidyl peptidase 4

Chain D:




V619
Y631
G632
G633
T636
A652
V653
A654
P655
V656
S657
R658
R669
Y670
M671
E677
R684
T687
V688
L702
I703
H704
G705
T706
N710
F713
S716
A717
V726
G727
V728
Q731
A732
M733
W734
Y735
T736
F758
L765
P766

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	122.09Å 123.01Å 144.65Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	32.80 – 2.49 32.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.80-2.49) 98.3 (32.82-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.244 0.238 , 0.276	Depositor DCC
R_{free} test set	6729 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.2	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 133885 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24805	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, B2Y

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	0.45	0/6111	0.62	1/8311 (0.0%)
1	B	0.44	0/6138	0.62	1/8348 (0.0%)
1	C	0.44	0/6111	0.61	1/8311 (0.0%)
1	D	0.42	0/6100	0.58	0/8296
All	All	0.44	0/24460	0.61	3/33266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	415	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	415	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	415	LEU	CA-CB-CG	5.13	127.11	115.30

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	5935	0	5657	72	0
1	B	5965	0	5672	63	0
1	C	5936	0	5660	65	0
1	D	5929	0	5651	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	56	0	52	0	0
2	B	56	0	52	1	0
2	C	28	0	26	0	0
2	D	28	0	26	1	0
3	A	56	0	50	0	0
3	B	28	0	25	1	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	206	0	0	2	0
5	B	191	0	0	0	0
5	C	189	0	0	1	0
5	D	90	0	0	0	0
All	All	24805	0	22973	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.42	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.14	0.93
1:A:153:GLN:HE22	1:A:170:ASN:H	1.18	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.14	0.90
1:C:54:ARG:HH21	1:C:54:ARG:HG2	1.39	0.88
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.56	0.88
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.71	0.87
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.58	0.85
1:D:153:GLN:HE22	1:D:170:ASN:H	1.22	0.84
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.88	0.83
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.59	0.82
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.82
1:A:325:MET:CE	1:A:327:ILE:HD11	2.11	0.81
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.64	0.79
1:C:434:ILE:HD11	1:C:439:TYR:HB2	1.67	0.74
1:A:129:THR:HG23	1:A:151:ASN:HA	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.73	0.70
1:D:179:ASN:H	1:D:179:ASN:HD22	1.42	0.67
1:A:129:THR:CG2	1:A:151:ASN:HA	2.25	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.79	0.64
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.92	0.64
1:B:36:HIS:O	1:B:37:HIS:HB2	1.98	0.63
1:B:614:SER:HA	1:B:619:VAL:HB	1.79	0.63
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.63
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.23	0.62
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.80	0.62
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.82	0.62
1:C:153:GLN:NE2	1:C:170:ASN:H	1.94	0.62
1:D:147:ARG:HE	2:D:801:NAG:H83	1.66	0.61
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.65	0.61
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.61
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.36	0.60
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.92	0.60
1:D:564:ALA:HB1	1:D:575:VAL:HG11	1.84	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:D:155:VAL:HG12	1:D:166:TYR:HB3	1.85	0.59
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.85	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:B:711:VAL:CG2	4:B:800:B2Y:H11	2.32	0.58
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.84	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.58
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.84	0.58
1:C:472:CYS:O	1:C:478:PRO:HA	2.04	0.57
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.67	0.57
1:D:522:THR:HB	1:D:524:PHE:CE2	2.40	0.57
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.86	0.57
1:D:382:ARG:H	1:D:403:GLU:HG2	1.69	0.57
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.87	0.56
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.86	0.56
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.40	0.56
1:C:152:THR:HG21	1:C:155:VAL:HG13	1.88	0.55
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.88	0.55
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.71	0.55
1:D:78:VAL:HG22	1:D:89:PHE:HB2	1.88	0.55
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.89	0.55
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLN:HE22	1:C:170:ASN:N	1.95	0.54
1:B:343:ARG:HD3	1:B:389:ILE:CG2	2.32	0.54
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.54
1:B:89:PHE:HE1	1:B:107:ILE:HD12	1.73	0.54
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.54
1:D:614:SER:HA	1:D:619:VAL:HB	1.89	0.53
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.74	0.53
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.39	0.53
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.89	0.53
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.90	0.52
1:A:135:TYR:HE2	1:A:140:ARG:HG2	1.74	0.52
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.52
1:A:170:ASN:N	1:A:170:ASN:HD22	2.08	0.51
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.92	0.51
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.40	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.91	0.51
1:B:179:ASN:H	1:B:179:ASN:HD22	1.57	0.51
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.51
1:D:453:ARG:NH2	1:D:477:LEU:O	2.43	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.46	0.51
1:B:147:ARG:HE	2:B:802:NAG:H83	1.75	0.51
1:C:369:ASN:C	1:C:389:ILE:HG12	2.32	0.51
1:C:369:ASN:O	1:C:389:ILE:HG12	2.11	0.50
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.50
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.27	0.50
1:D:598:LEU:HG	1:D:631:TYR:OH	2.12	0.49
1:D:334:SER:HB2	1:D:336:ARG:H	1.77	0.49
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.93	0.49
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.49
1:C:54:ARG:NH2	1:C:54:ARG:HG2	2.16	0.49
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.49
1:B:79:PHE:HA	1:B:86:SER:HB3	1.94	0.49
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.49
1:B:47:ASP:HA	1:B:52:THR:OG1	2.12	0.49
1:B:80:ASN:HD22	1:B:83:TYR:H	1.59	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.13	0.49
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.13	0.49
1:C:327:ILE:HD13	1:C:389:ILE:HG23	1.95	0.48
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.13	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:OD1	1:D:91:GLU:HG3	2.12	0.48
1:C:473:SER:O	1:C:474:GLY:O	2.32	0.48
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.95	0.48
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.14	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.47
1:B:473:SER:O	1:B:474:GLY:O	2.32	0.47
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.13	0.47
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.48	0.47
1:C:179:ASN:HD22	1:C:179:ASN:C	2.18	0.47
1:B:71:LYS:HA	1:B:75:ASN:O	2.14	0.47
1:A:153:GLN:HE22	1:A:170:ASN:N	2.00	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.49	0.47
3:B:804:NAG:H62	3:B:805:NAG:N2	2.30	0.47
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.96	0.47
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.80	0.47
1:D:80:ASN:HD22	1:D:83:TYR:HB2	1.80	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.96	0.47
1:D:435:GLN:HE21	1:D:437:SER:HG	1.63	0.47
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.47
1:C:303:VAL:HG22	1:C:313:LEU:HD12	1.97	0.47
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.49	0.46
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.97	0.46
1:D:158:SER:OG	1:D:163:LYS:HB2	2.15	0.46
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.46
1:A:685:ASN:ND2	5:A:866:HOH:O	2.48	0.46
1:D:710:ASN:C	1:D:710:ASN:HD22	2.19	0.46
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.97	0.46
1:C:55:LEU:HD23	1:C:500:LEU:HD22	1.98	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.46
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.98	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.98	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.98	0.46
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.31	0.45
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.80	0.45
1:D:405:ILE:HG12	1:D:419:SER:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.45
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.45
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.98	0.45
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.52	0.45
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.45
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.45
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.47	0.45
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.82	0.45
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.45
1:C:410:LEU:HD22	1:C:411:THR:O	2.16	0.45
1:B:153:GLN:NE2	1:B:170:ASN:H	2.06	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.52	0.45
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.94	0.45
1:D:129:THR:HG23	1:D:151:ASN:HA	1.98	0.45
1:D:731:GLN:HG3	1:D:758:PHE:HE1	1.82	0.44
1:A:135:TYR:CE2	1:A:140:ARG:HA	2.52	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.44
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.99	0.44
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.15	0.44
1:C:614:SER:HA	1:C:619:VAL:HB	2.00	0.44
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.44
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.52	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.00	0.44
1:B:378:GLU:H	1:B:378:GLU:CD	2.21	0.44
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.82	0.44
1:B:75:ASN:HD21	1:B:92:ASN:HD22	1.66	0.43
1:D:517:ILE:HD11	1:D:578:PHE:CE1	2.53	0.43
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.54	0.43
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.00	0.43
1:B:405:ILE:HG12	1:B:419:SER:HA	2.00	0.43
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.01	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.43
1:C:544:LEU:HD23	1:C:626:ILE:HD12	2.00	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.54	0.43
1:A:473:SER:O	1:A:474:GLY:O	2.36	0.43
1:D:291:ALA:O	1:D:295:ILE:HG23	2.18	0.43
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.54	0.43
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.54	0.43
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ARG:HA	1:A:670:TYR:O	2.19	0.43
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.53	0.43
1:C:148:ILE:HD11	1:C:164:LEU:HD21	2.01	0.43
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.58	0.43
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.54	0.42
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.49	0.42
1:A:72:GLN:HB2	1:A:77:LEU:HD21	2.01	0.42
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.54	0.42
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.19	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:C:418:ILE:HA	1:C:430:ASN:O	2.19	0.42
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.42
1:A:129:THR:HG22	5:A:1002:HOH:O	2.18	0.42
1:C:155:VAL:HG12	1:C:166:TYR:HB3	2.01	0.42
1:D:450:ASN:O	1:D:454:CYS:HB2	2.20	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.42
1:C:179:ASN:HD22	1:C:180:LEU:N	2.17	0.42
1:D:435:GLN:OE1	1:D:441:LYS:HD3	2.19	0.42
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.91	0.42
1:C:167:VAL:HA	1:C:171:ASP:O	2.20	0.41
1:B:70:TYR:CG	1:B:71:LYS:N	2.88	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.41
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:C:302:ASP:HB3	1:C:314:GLN:HB2	2.01	0.41
1:C:397:ILE:HD12	1:C:434:ILE:HD13	2.03	0.41
1:B:506:ASN:HB2	1:C:440:THR:CG2	2.49	0.41
1:A:378:GLU:CD	1:A:378:GLU:H	2.23	0.41
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.41
1:D:98:PHE:CD1	1:D:100:HIS:HB2	2.55	0.41
1:D:79:PHE:CD2	1:D:86:SER:HB3	2.54	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:A:458:SER:OG	1:A:471:ARG:HB3	2.21	0.41
1:D:598:LEU:HB2	1:D:671:MET:SD	2.60	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.55	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:TYR:HA	1:D:115:LEU:O	2.20	0.41
1:A:135:TYR:CE2	1:A:140:ARG:HG2	2.55	0.41
1:C:478:PRO:HB2	1:C:497:ASN:ND2	2.36	0.41
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.02	0.41
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.56	0.41
1:D:55:LEU:HD23	1:D:500:LEU:HD22	2.02	0.41
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.41
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.03	0.41
1:A:242:SER:OG	1:A:243:ASP:N	2.53	0.41
1:D:167:VAL:HA	1:D:171:ASP:O	2.21	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.77	0.41
1:B:598:LEU:O	1:B:682:HIS:NE2	2.52	0.41
1:A:154:TRP:CD2	1:A:212:SER:HB3	2.56	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HG	2.02	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.51	0.41
1:A:146:GLU:O	1:A:175:LYS:NZ	2.52	0.41
1:C:562:ASN:HB2	5:C:841:HOH:O	2.20	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.22	0.41
1:B:582:GLY:CA	1:B:594:ILE:HD12	2.50	0.40
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.51	0.40
1:C:484:SER:O	1:C:488:ASP:HA	2.20	0.40
1:A:546:VAL:HG12	1:A:627:TRP:O	2.21	0.40
1:D:164:LEU:HB3	1:D:175:LYS:HB2	2.03	0.40
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.40
1:A:158:SER:OG	1:A:163:LYS:HB2	2.22	0.40
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.57	0.40
1:B:63:ILE:HA	1:B:63:ILE:HD12	1.81	0.40
1:C:243:ASP:C	1:C:245:SER:N	2.75	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	721/740 (97%)	684 (95%)	36 (5%)	1 (0%)	56	78
1	B	725/740 (98%)	698 (96%)	25 (3%)	2 (0%)	46	68
1	C	721/740 (97%)	688 (95%)	31 (4%)	2 (0%)	46	68
1	D	720/740 (97%)	684 (95%)	34 (5%)	2 (0%)	46	68
All	All	2887/2960 (98%)	2754 (95%)	126 (4%)	7 (0%)	52	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	GLY
1	A	474	GLY
1	B	37	HIS
1	B	474	GLY
1	D	474	GLY
1	C	92	ASN
1	D	109	PRO

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	650/662 (98%)	611 (94%)	39 (6%)	24	43
1	B	652/662 (98%)	611 (94%)	41 (6%)	22	40
1	C	650/662 (98%)	614 (94%)	36 (6%)	27	48
1	D	649/662 (98%)	617 (95%)	32 (5%)	31	55
All	All	2601/2648 (98%)	2453 (94%)	148 (6%)	25	46

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	80	ASN
1	A	95	PHE
1	A	145	GLU
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	343	ARG
1	A	358[A]	ARG
1	A	358[B]	ARG
1	A	385	CYS
1	A	389	ILE
1	A	415	LEU
1	A	436	LEU
1	A	441	LYS
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	566	TYR
1	A	575	VAL
1	A	598	LEU
1	A	630	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	59	SER
1	B	61	ARG
1	B	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	129	THR
1	B	139	LYS
1	B	142	LEU
1	B	164	LEU
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	316	LEU
1	B	325	MET
1	B	360	SER
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	464	GLU
1	B	473	SER
1	B	477	LEU
1	B	482	LEU
1	B	504	LEU
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	566	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	627	TRP
1	B	660	GLU
1	B	685	ASN
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	80	ASN
1	C	129	THR
1	C	170	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	ASN
1	C	243	ASP
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET
1	C	385	CYS
1	C	395	THR
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	434	ILE
1	C	436	LEU
1	C	441	LYS
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	538	LYS
1	C	575	VAL
1	C	589	LYS
1	C	615	LYS
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	D	51	ASN
1	D	56	LYS
1	D	78	VAL
1	D	90	LEU
1	D	109	PRO
1	D	129	THR
1	D	137	LEU
1	D	140	ARG
1	D	142	LEU
1	D	170	ASN
1	D	179	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	280	THR
1	D	316	LEU
1	D	365	THR
1	D	385	CYS
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU
1	D	453	ARG
1	D	482	LEU
1	D	492	ARG
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	575	VAL
1	D	598	LEU
1	D	688	VAL
1	D	704	HIS
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	80	ASN
1	B	92	ASN
1	B	123	GLN
1	B	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	430	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	51	ASN
1	C	80	ASN
1	C	100	HIS
1	C	123	GLN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	505	GLN
1	C	697	GLN
1	C	710	ASN
1	C	748	HIS
1	D	80	ASN
1	D	138	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	430	ASN
1	D	455	GLN
1	D	508	GLN
1	D	572	ASN
1	D	592	HIS
1	D	621	ASN
1	D	710	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	748	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

10 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	804	1,3	14,14,15	0.58	0	15,19,21	0.74	0
3	NAG	A	805	3	14,14,15	0.44	0	15,19,21	1.09	1 (6%)
3	NAG	A	806	1,3	14,14,15	0.52	0	15,19,21	1.35	2 (13%)
3	NAG	A	807	3	14,14,15	0.55	0	15,19,21	0.74	0
3	NAG	B	804	1,3	14,14,15	0.61	0	15,19,21	1.02	0
3	NAG	B	805	3	14,14,15	0.51	0	15,19,21	0.91	0
3	NAG	C	803	1,3	14,14,15	0.61	0	15,19,21	0.94	0
3	NAG	C	804	3	14,14,15	0.60	0	15,19,21	1.22	2 (13%)
3	NAG	D	802	1,3	14,14,15	0.43	0	15,19,21	0.95	1 (6%)
3	NAG	D	803	3	14,14,15	0.58	0	15,19,21	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	807	3	-	0/6/23/26	0/1/1/1
3	NAG	B	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	805	3	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	804	3	-	0/6/23/26	0/1/1/1
3	NAG	D	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	NAG	C2-N2-C7	-2.55	119.76	123.04
3	A	805	NAG	C1-O5-C5	2.02	114.81	112.25
3	C	804	NAG	C3-C4-C5	2.26	114.13	110.20
3	D	802	NAG	C1-O5-C5	2.63	115.59	112.25
3	A	806	NAG	C1-O5-C5	3.06	116.13	112.25
3	C	804	NAG	C4-C3-C2	3.51	116.68	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	NAG	1	0
3	B	805	NAG	1	0

5.6 Ligand geometry (i)

16 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	B2Y	A	800	-	15,15,15	0.46	0	18,19,19	0.72	0
2	NAG	A	801	1	14,14,15	0.56	0	15,19,21	1.54	1 (6%)
2	NAG	A	802	1	14,14,15	0.55	0	15,19,21	1.58	1 (6%)
2	NAG	A	803	1	14,14,15	0.57	0	15,19,21	1.01	1 (6%)
2	NAG	A	808	1	14,14,15	0.55	0	15,19,21	1.49	1 (6%)
4	B2Y	B	800	-	15,15,15	0.48	0	18,19,19	0.54	0
2	NAG	B	801	1	14,14,15	0.74	1 (7%)	15,19,21	1.32	2 (13%)
2	NAG	B	802	1	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
2	NAG	B	803	1	14,14,15	0.60	0	15,19,21	1.29	1 (6%)
2	NAG	B	806	1	14,14,15	0.53	0	15,19,21	1.81	1 (6%)
4	B2Y	C	800	-	15,15,15	0.46	0	18,19,19	0.64	0
2	NAG	C	801	1	14,14,15	0.48	0	15,19,21	1.53	1 (6%)
2	NAG	C	802	1	14,14,15	0.61	0	15,19,21	1.31	1 (6%)
4	B2Y	D	800	-	15,15,15	0.45	0	18,19,19	0.57	0
2	NAG	D	801	1	14,14,15	0.57	0	15,19,21	1.14	1 (6%)
2	NAG	D	804	1	14,14,15	0.75	1 (7%)	15,19,21	1.55	2 (13%)

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	B2Y	A	800	-	-	0/6/6/6	0/2/2/2
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
4	B2Y	B	800	-	-	0/6/6/6	0/2/2/2
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
4	B2Y	C	800	-	-	0/6/6/6	0/2/2/2
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
4	B2Y	D	800	-	-	0/6/6/6	0/2/2/2
2	NAG	D	801	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	D	804	1	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	NAG	C1-C2	2.06	1.55	1.52
2	D	804	NAG	C1-C2	2.41	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	804	NAG	C3-C4-C5	-2.39	106.03	110.20
2	B	801	NAG	O5-C5-C6	2.30	112.32	107.35
2	A	803	NAG	C4-C3-C2	2.37	114.91	111.23
2	D	801	NAG	C1-O5-C5	2.76	115.75	112.25
2	B	801	NAG	C4-C3-C2	2.94	115.81	111.23
2	C	802	NAG	C4-C3-C2	3.45	116.59	111.23
2	D	804	NAG	C1-O5-C5	4.06	117.40	112.25
2	B	802	NAG	C1-O5-C5	4.21	117.60	112.25
2	B	803	NAG	C1-O5-C5	4.22	117.60	112.25
2	C	801	NAG	C1-O5-C5	4.68	118.19	112.25
2	A	808	NAG	C1-O5-C5	4.92	118.49	112.25
2	A	801	NAG	C1-O5-C5	5.12	118.75	112.25
2	A	802	NAG	C1-O5-C5	5.75	119.54	112.25
2	B	806	NAG	C1-O5-C5	6.02	119.89	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	804	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	B2Y	1	0
2	B	802	NAG	1	0
2	D	801	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	724/740 (97%)	0.67	87 (12%) 6 6	37, 48, 68, 104	0
1	B	729/740 (98%)	0.39	48 (6%) 22 24	36, 47, 67, 83	0
1	C	724/740 (97%)	0.72	99 (13%) 4 4	37, 48, 69, 101	0
1	D	724/740 (97%)	0.82	132 (18%) 2 2	36, 51, 69, 107	0
All	All	2901/2960 (98%)	0.65	366 (12%) 5 5	36, 48, 68, 107	0

All (366) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	8.5
1	D	83	TYR	8.1
1	C	135	TYR	7.8
1	C	279	VAL	7.4
1	D	93	SER	7.3
1	C	93	SER	6.6
1	D	94	THR	6.4
1	C	94	THR	6.3
1	C	99	GLY	5.9
1	A	92	ASN	5.8
1	A	88	VAL	5.7
1	D	77	LEU	5.6
1	A	135	TYR	5.5
1	D	386	TYR	5.4
1	C	96	ASP	5.3
1	D	414	TYR	5.1
1	A	140	ARG	5.0
1	C	83	TYR	4.8
1	C	92	ASN	4.8
1	C	141	GLN	4.8
1	C	280	THR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	ASP	4.8
1	B	81	ALA	4.7
1	A	86	SER	4.7
1	B	518	ILE	4.7
1	B	88	VAL	4.6
1	D	88	VAL	4.6
1	D	734	TRP	4.6
1	D	412	SER	4.5
1	D	330	TYR	4.5
1	D	333	SER	4.5
1	D	518	ILE	4.5
1	A	95	PHE	4.4
1	D	487	ASN	4.4
1	D	81	ALA	4.4
1	B	87	SER	4.4
1	B	86	SER	4.4
1	D	55	LEU	4.4
1	C	102	ILE	4.4
1	A	635	VAL	4.4
1	A	97	GLU	4.4
1	A	333	SER	4.3
1	D	97	GLU	4.3
1	C	81	ALA	4.3
1	C	187	TRP	4.3
1	D	78	VAL	4.2
1	A	702	LEU	4.2
1	A	332	GLU	4.2
1	D	441	LYS	4.1
1	B	70	TYR	4.1
1	D	505	GLN	4.1
1	A	138	ASN	4.1
1	C	392	LYS	4.0
1	C	340	LEU	3.9
1	A	98	PHE	3.9
1	D	85	ASN	3.9
1	D	436	LEU	3.9
1	D	334	SER	3.9
1	C	702	LEU	3.9
1	D	468	TYR	3.9
1	C	489	LYS	3.8
1	C	734	TRP	3.8
1	D	62	TRP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	322	TYR	3.8
1	D	713	PHE	3.8
1	C	97	GLU	3.8
1	A	93	SER	3.8
1	D	498	SER	3.8
1	D	766	PRO	3.7
1	B	72	GLN	3.7
1	C	467	TYR	3.7
1	D	399	LYS	3.7
1	D	439	TYR	3.7
1	D	413	ASP	3.7
1	D	486	VAL	3.7
1	D	86	SER	3.7
1	D	435	GLN	3.7
1	A	700	TYR	3.6
1	D	467	TYR	3.6
1	A	69	LEU	3.6
1	D	366	LEU	3.6
1	A	636	THR	3.6
1	D	84	GLY	3.6
1	A	81	ALA	3.6
1	D	96	ASP	3.6
1	D	100	HIS	3.6
1	C	332	GLU	3.5
1	A	94	THR	3.5
1	D	397	ILE	3.5
1	D	56	LYS	3.5
1	C	474	GLY	3.4
1	A	651	ILE	3.4
1	B	546	VAL	3.4
1	A	655	PRO	3.4
1	C	487	ASN	3.4
1	A	652	ALA	3.4
1	C	390	ASP	3.4
1	A	634	TYR	3.4
1	A	713	PHE	3.4
1	A	656	VAL	3.3
1	A	279	VAL	3.3
1	D	706	THR	3.3
1	A	626	ILE	3.3
1	D	340	LEU	3.3
1	C	506	ASN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	135	TYR	3.2
1	A	701	LEU	3.2
1	D	332	GLU	3.2
1	C	732	ALA	3.2
1	D	92	ASN	3.2
1	D	66	HIS	3.2
1	C	652	ALA	3.2
1	D	464	GLU	3.2
1	C	719	ILE	3.2
1	D	98	PHE	3.2
1	A	87	SER	3.2
1	A	719	ILE	3.2
1	C	486	VAL	3.2
1	D	491	LEU	3.2
1	A	84	GLY	3.2
1	A	637	SER	3.2
1	C	80	ASN	3.1
1	B	734	TRP	3.1
1	C	636	THR	3.1
1	C	713	PHE	3.1
1	A	141	GLN	3.1
1	C	142	LEU	3.1
1	D	331	ASP	3.1
1	B	90	LEU	3.1
1	B	78	VAL	3.1
1	A	703	ILE	3.1
1	B	83	TYR	3.0
1	C	82	GLU	3.0
1	A	716	SER	3.0
1	B	77	LEU	3.0
1	D	483	HIS	3.0
1	C	717	ALA	3.0
1	D	437	SER	3.0
1	D	652	ALA	3.0
1	C	536	LYS	3.0
1	B	89	PHE	3.0
1	A	627	TRP	3.0
1	D	80	ASN	3.0
1	D	466	LYS	2.9
1	A	732	ALA	2.9
1	C	98	PHE	2.9
1	D	327	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	656	VAL	2.9
1	D	91	GLU	2.9
1	D	702	LEU	2.9
1	C	505	GLN	2.9
1	D	615	LYS	2.9
1	D	339	CYS	2.9
1	D	521	GLU	2.9
1	D	655	PRO	2.9
1	D	372	TYR	2.9
1	C	716	SER	2.9
1	D	338	ASN	2.9
1	C	388	GLN	2.9
1	C	91	GLU	2.8
1	D	716	SER	2.8
1	C	62	TRP	2.8
1	B	71	LYS	2.8
1	B	676	PRO	2.8
1	D	141	GLN	2.8
1	C	138	ASN	2.8
1	D	335	GLY	2.8
1	A	72	GLN	2.8
1	D	703	ILE	2.8
1	C	276	LEU	2.8
1	C	140	ARG	2.8
1	C	391	LYS	2.8
1	C	700	TYR	2.8
1	C	482	LEU	2.8
1	A	711	VAL	2.8
1	C	277	SER	2.8
1	A	77	LEU	2.8
1	A	632	GLY	2.7
1	D	68	TYR	2.7
1	D	546	VAL	2.7
1	A	654	ALA	2.7
1	A	717	ALA	2.7
1	C	231	THR	2.7
1	D	365	THR	2.7
1	D	636	THR	2.7
1	B	82	GLU	2.7
1	C	393	ASP	2.7
1	D	389	ILE	2.7
1	A	640	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	392	LYS	2.7
1	D	95	PHE	2.7
1	A	180	LEU	2.7
1	C	100	HIS	2.7
1	B	99	GLY	2.7
1	D	342	ALA	2.7
1	D	499	ALA	2.7
1	D	67	GLU	2.6
1	C	637	SER	2.6
1	D	411	THR	2.6
1	A	715	GLN	2.6
1	C	336	ARG	2.6
1	C	139	LYS	2.6
1	D	523	LYS	2.6
1	A	704	HIS	2.6
1	B	628	GLY	2.6
1	A	392	LYS	2.6
1	D	442	VAL	2.6
1	D	370	SER	2.6
1	D	54	ARG	2.6
1	D	380	GLY	2.6
1	D	633	GLY	2.6
1	A	688	VAL	2.6
1	B	703	ILE	2.6
1	D	440	THR	2.6
1	A	546	VAL	2.5
1	B	733	MET	2.5
1	D	733	MET	2.5
1	D	717	ALA	2.5
1	B	653	VAL	2.5
1	C	537	SER	2.5
1	D	677	GLU	2.5
1	C	72	GLN	2.5
1	D	656	VAL	2.5
1	D	432	TYR	2.5
1	B	713	PHE	2.5
1	D	393	ASP	2.5
1	C	711	VAL	2.5
1	B	702	LEU	2.5
1	C	333	SER	2.5
1	B	636	THR	2.5
1	B	521	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	452	GLU	2.4
1	A	63	ILE	2.4
1	A	628	GLY	2.4
1	A	650	GLY	2.4
1	A	142	LEU	2.4
1	D	415	LEU	2.4
1	A	280	THR	2.4
1	A	638	MET	2.4
1	C	655	PRO	2.4
1	A	91	GLU	2.4
1	A	657	SER	2.4
1	C	87	SER	2.4
1	B	241	TYR	2.4
1	D	70	TYR	2.4
1	D	704	HIS	2.4
1	C	113	PHE	2.4
1	D	222	PHE	2.4
1	A	474	GLY	2.4
1	A	90	LEU	2.4
1	A	543	LEU	2.4
1	B	656	VAL	2.4
1	C	546	VAL	2.4
1	C	715	GLN	2.4
1	A	103	ASN	2.4
1	A	631	TYR	2.4
1	B	633	GLY	2.4
1	D	41	LYS	2.4
1	A	231	THR	2.4
1	B	577	SER	2.4
1	B	632	GLY	2.3
1	C	54	ARG	2.3
1	B	544	LEU	2.3
1	C	115	LEU	2.3
1	A	733	MET	2.3
1	C	703	ILE	2.3
1	D	71	LYS	2.3
1	D	346	ILE	2.3
1	A	99	GLY	2.3
1	C	688	VAL	2.3
1	D	416	TYR	2.3
1	B	711	VAL	2.3
1	D	75	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	633	GLY	2.3
1	D	72	GLN	2.3
1	D	388	GLN	2.3
1	D	390	ASP	2.3
1	A	71	LYS	2.3
1	B	79	PHE	2.3
1	A	300	LEU	2.3
1	C	84	GLY	2.3
1	A	502	LYS	2.3
1	A	625	ALA	2.3
1	C	651	ILE	2.3
1	D	63	ILE	2.3
1	C	483	HIS	2.3
1	C	704	HIS	2.3
1	C	341	VAL	2.3
1	C	76	ILE	2.2
1	D	384	ILE	2.2
1	B	631	TYR	2.2
1	D	735	TYR	2.2
1	D	392	LYS	2.2
1	A	506	ASN	2.2
1	C	338	ASN	2.2
1	D	484	SER	2.2
1	D	79	PHE	2.2
1	A	214	LEU	2.2
1	C	521	GLU	2.2
1	A	299	TYR	2.2
1	C	635	VAL	2.2
1	D	653	VAL	2.2
1	D	276	LEU	2.2
1	D	500	LEU	2.2
1	A	78	VAL	2.2
1	D	336	ARG	2.2
1	D	684	ARG	2.2
1	C	89	PHE	2.2
1	A	316	LEU	2.2
1	A	66	HIS	2.2
1	B	704	HIS	2.2
1	C	101	SER	2.2
1	C	491	LEU	2.2
1	D	410	LEU	2.2
1	C	468	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	348	MET	2.2
1	B	76	ILE	2.2
1	C	90	LEU	2.2
1	D	736	THR	2.2
1	A	360	SER	2.1
1	A	467	TYR	2.1
1	C	63	ILE	2.1
1	B	333	SER	2.1
1	C	278	SER	2.1
1	D	391	LYS	2.1
1	D	400	GLY	2.1
1	D	87	SER	2.1
1	A	358[A]	ARG	2.1
1	D	82	GLU	2.1
1	D	90	LEU	2.1
1	A	354	VAL	2.1
1	D	654	ALA	2.1
1	D	438	ASP	2.1
1	B	142	LEU	2.1
1	C	640	LEU	2.1
1	C	695	PHE	2.1
1	B	36	HIS	2.1
1	C	706	THR	2.1
1	A	342	ALA	2.1
1	A	603	VAL	2.1
1	B	651	ILE	2.1
1	C	414	TYR	2.1
1	D	58	TYR	2.1
1	C	650	GLY	2.1
1	C	485	SER	2.1
1	B	652	ALA	2.1
1	D	503	MET	2.1
1	B	97	GLU	2.1
1	B	547	TYR	2.1
1	A	544	LEU	2.1
1	D	449	LEU	2.1
1	D	433	LYS	2.0
1	D	538	LYS	2.0
1	C	504	LEU	2.0
1	C	634	TYR	2.0
1	D	417	TYR	2.0
1	A	144	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	52	THR	2.0
1	D	401	THR	2.0
1	C	85	ASN	2.0
1	C	79	PHE	2.0
1	C	75	ASN	2.0
1	B	141	GLN	2.0
1	B	545	ASP	2.0
1	A	659	TRP	2.0
1	C	118	TYR	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, 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
3	NAG	B	804	14/15	0.87	0.22	1.74	67,69,73,77	0
3	NAG	A	804	14/15	0.94	0.21	0.31	58,60,62,66	0
3	NAG	C	803	14/15	0.90	0.19	-0.05	63,65,68,72	0
3	NAG	D	802	14/15	0.92	0.16	-0.85	55,58,61,63	0
3	NAG	B	805	14/15	0.82	0.43	-	80,82,83,83	0
3	NAG	C	804	14/15	0.81	0.34	-	73,76,78,78	0
3	NAG	A	806	14/15	0.76	0.24	-	73,76,79,80	0
3	NAG	A	805	14/15	0.89	0.30	-	68,70,71,71	0
3	NAG	D	803	14/15	0.83	0.26	-	67,68,72,72	0
3	NAG	A	807	14/15	0.82	0.35	-	83,84,85,85	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, 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	A	808	14/15	0.86	0.30	3.93	61,63,64,64	0
2	NAG	C	802	14/15	0.88	0.32	3.74	68,70,74,74	0
4	B2Y	B	800	14/14	0.88	0.28	1.20	60,62,63,64	0
4	B2Y	C	800	14/14	0.89	0.25	0.62	50,54,55,55	0
2	NAG	A	801	14/15	0.64	0.32	0.23	72,73,74,74	0
4	B2Y	A	800	14/14	0.88	0.24	0.10	53,56,58,58	0
4	B2Y	D	800	14/14	0.93	0.17	-0.10	42,44,46,46	0
2	NAG	B	802	14/15	0.89	0.20	-	63,64,66,66	0
2	NAG	A	802	14/15	0.77	0.30	-	65,66,68,68	0
2	NAG	B	803	14/15	0.81	0.33	-	63,65,68,68	0
2	NAG	B	806	14/15	0.80	0.14	-	67,69,73,74	0
2	NAG	C	801	14/15	0.77	0.20	-	55,55,56,57	0
2	NAG	A	803	14/15	0.72	0.33	-	71,73,76,77	0
2	NAG	D	801	14/15	0.86	0.19	-	58,60,62,63	0
2	NAG	B	801	14/15	0.73	0.23	-	78,79,80,80	0
2	NAG	D	804	14/15	0.82	0.20	-	78,80,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.