Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:08 PM GMT

PDB ID	:	1S78
Title	:	Insights into ErbB signaling from the structure of the ErbB2-pertuzumab complex
Authors	:	Franklin, M.C.; Carey, K.D.; Vajdos, F.F.; Leahy, D.J.; de Vos, A.M.; Sliwkowski, M.X.
Deposited on	:	2004-01-29
Resolution	:	3.25 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:

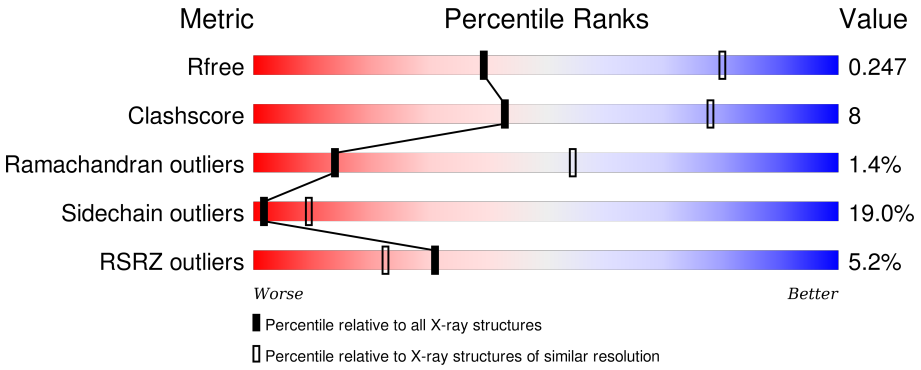
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	624	3% 64% 21% 5% 11%
1	B	624	2% 63% 23% 5% 9%
2	C	214	16% 60% 35% 5%
2	E	214	% 71% 25% •
3	D	226	12% 59% 33% 6% •

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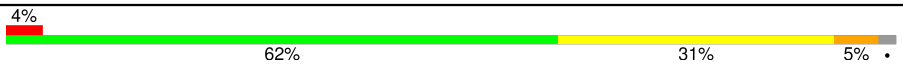
Mol	Chain	Length	Quality of chain
3	F	226	

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	NAG	A	1001	X	-	-	X
4	NAG	B	1001	X	-	-	-
6	NAG	B	1003	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15481 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 Receptor protein-tyrosine kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			
1	B	568	Total	C	N	O	S	0	0	0
			4381	2723	788	821	49			

- Molecule 2 is a protein called Pertuzumab Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1657	1043	272	336	6			
2	E	214	Total	C	N	O	S	0	0	0
			1657	1043	272	336	6			

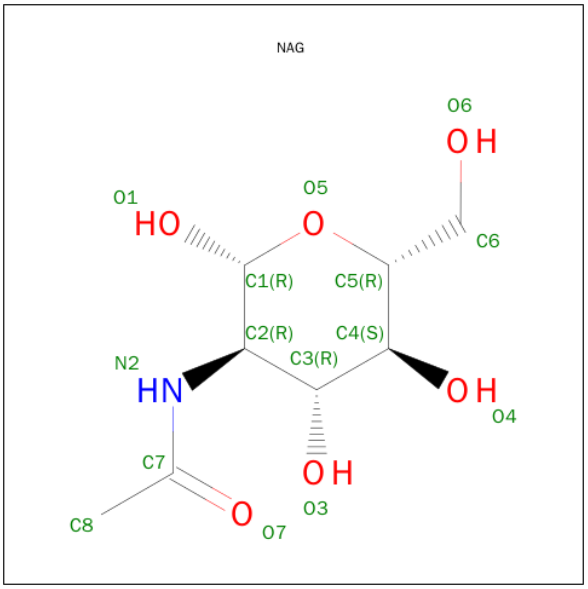
- Molecule 3 is a protein called Pertuzumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	222	Total	C	N	O	S	0	0	0
			1665	1051	280	327	7			
3	F	222	Total	C	N	O	S	0	0	0
			1665	1051	280	327	7			

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

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

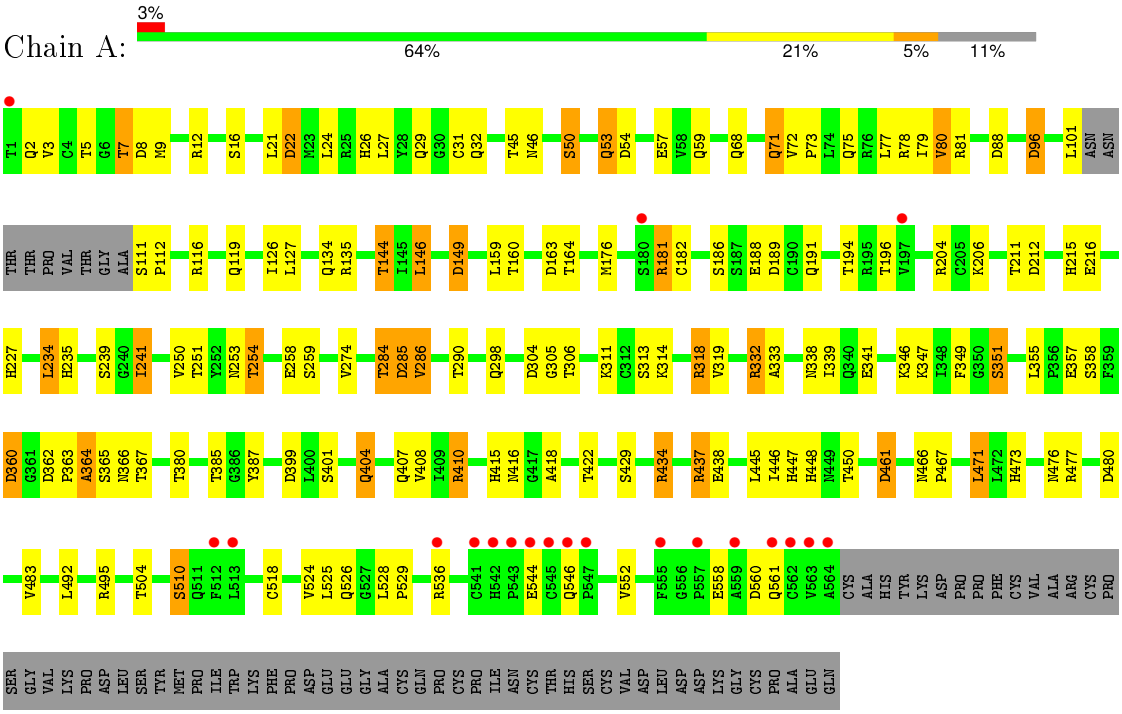
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		

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.

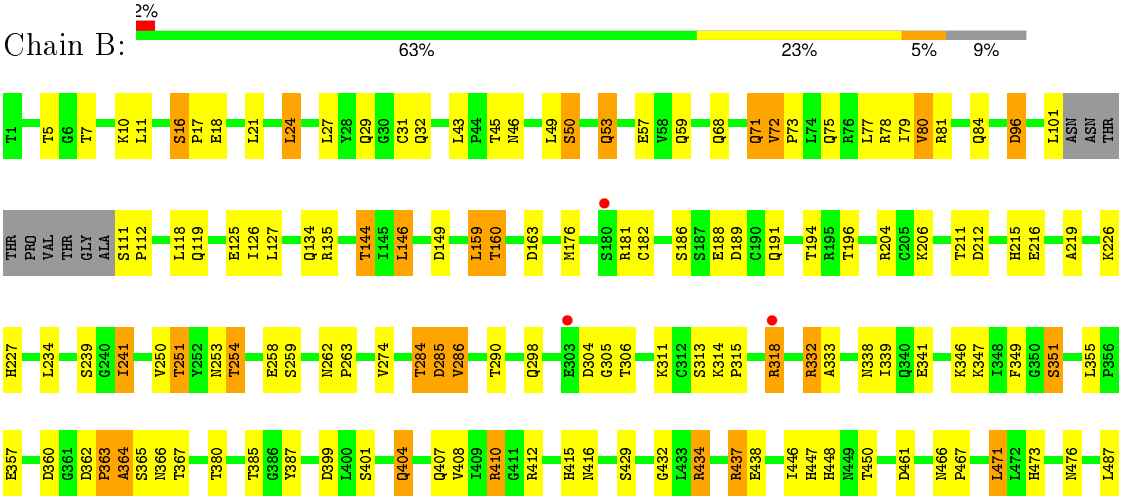
- Molecule 1: Receptor protein-tyrosine kinase erbB-2

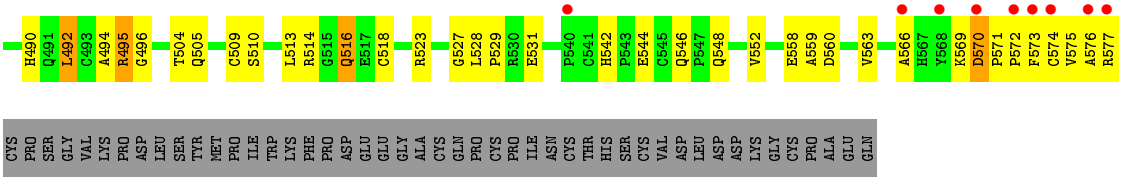
Chain A:



- Molecule 1: Receptor protein-tyrosine kinase erbB-2

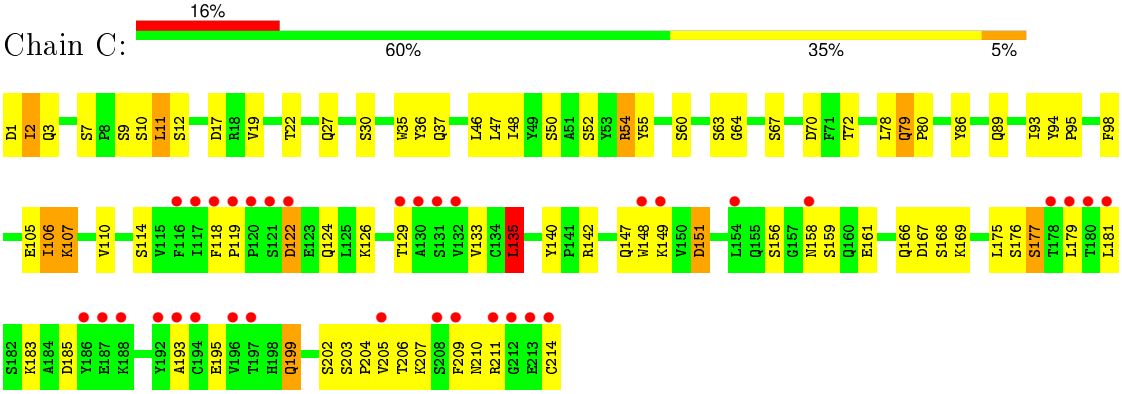
Chain B:





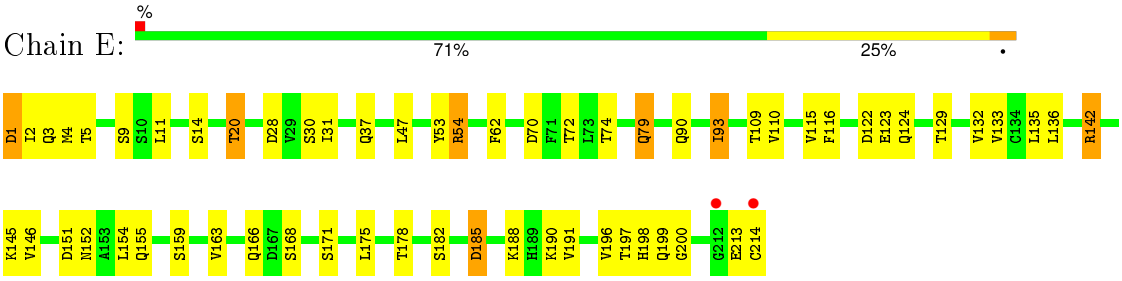
- Molecule 2: Pertuzumab Fab light chain

Chain C:



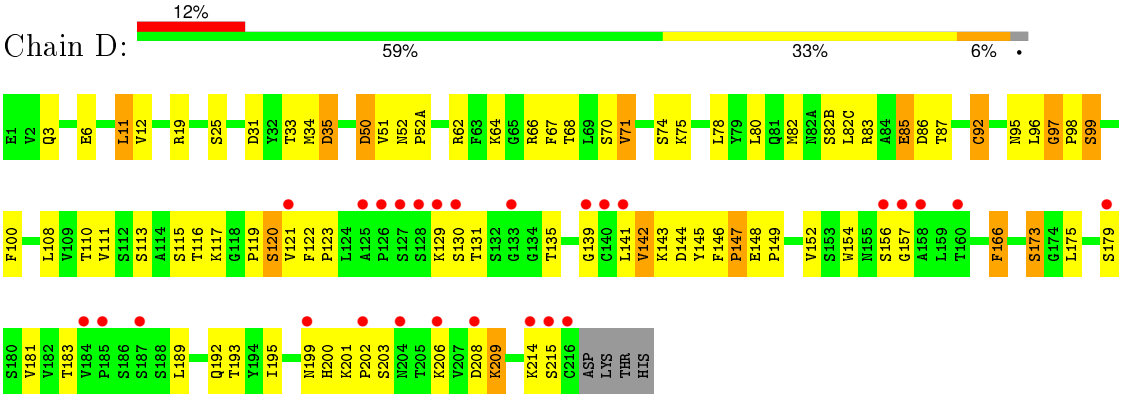
- Molecule 2: Pertuzumab Fab light chain

Chain E:



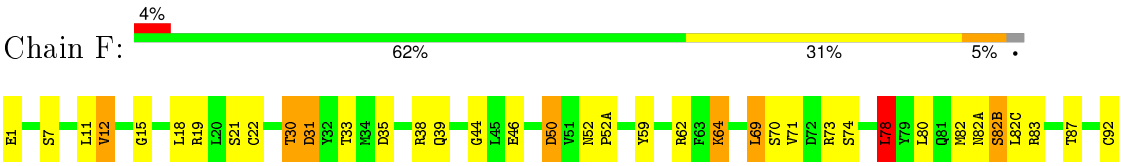
- Molecule 3: Pertuzumab Fab heavy chain

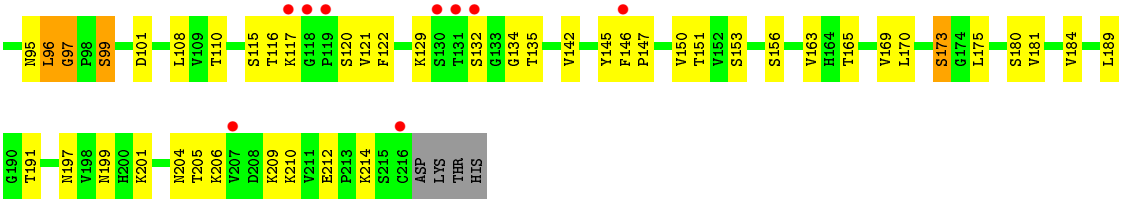
Chain D:



- Molecule 3: Pertuzumab Fab heavy chain

Chain F:




N95
L96
G97
P98
S99
D101
L108
V109
T110
S115
T116
K117
G118
P119
S120
V121
F122
K129
S130
T131
S132
G133
G134
T135
V142
Y145
F146
P147
V150
T151
V152
S153
S156
V163
H164
T165
V169
L170
S173
G174
L175
S180
V181
V184
L189
G190
T191
N197
V198
N199
H200
K201
N204
T205
K206
V207
D208
K209
K210
V211
E212
P213
K214
S215
C216
ASP
LYS
THR
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.41Å 139.41Å 356.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.25 29.85 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.25) 99.9 (29.85-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.268 0.210 , 0.247	Depositor DCC
R_{free} test set	2835 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	81.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 56261 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15481	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: BMA, NAG

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	0.43	0/4374	0.77	15/5950 (0.3%)
1	B	0.44	0/4483	0.75	10/6099 (0.2%)
2	C	0.38	0/1695	0.71	6/2301 (0.3%)
2	E	0.39	0/1695	0.71	5/2301 (0.2%)
3	D	0.39	0/1706	0.72	5/2324 (0.2%)
3	F	0.42	0/1706	0.76	4/2324 (0.2%)
All	All	0.42	0/15659	0.75	45/21299 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	1	0
4	B	1	0
All	All	2	0

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	A	318	ARG	NE-CZ-NH1	-9.13	115.73	120.30
3	F	97	GLY	N-CA-C	-8.23	92.52	113.10
3	D	97	GLY	N-CA-C	-7.86	93.45	113.10
1	B	318	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	B	318	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	E	185	ASP	CB-CG-OD2	6.36	124.02	118.30
3	F	31	ASP	CB-CG-OD2	6.34	124.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	96	ASP	CB-CG-OD2	6.32	123.99	118.30
3	D	50	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	212	ASP	CB-CG-OD2	6.19	123.87	118.30
3	D	35	ASP	CB-CG-OD2	6.01	123.71	118.30
3	F	78	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	8	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	22	ASP	CB-CG-OD2	5.61	123.35	118.30
2	E	28	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	399	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	304	ASP	CB-CG-OD2	5.40	123.16	118.30
2	E	1	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	285	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	88	ASP	CB-CG-OD2	5.31	123.08	118.30
2	E	151	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	149	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	399	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	570	ASP	CB-CG-OD2	5.26	123.03	118.30
2	C	167	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	96	ASP	CB-CG-OD2	5.19	122.97	118.30
2	C	185	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	560	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	360	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	480	ASP	CB-CG-OD2	5.15	122.94	118.30
2	C	122	ASP	CB-CG-OD2	5.13	122.92	118.30
3	D	208	ASP	CB-CG-OD2	5.12	122.91	118.30
3	F	50	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	17	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	285	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	54	ASP	CB-CG-OD2	5.07	122.86	118.30
2	E	122	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	159	LEU	CA-CB-CG	5.06	126.94	115.30
2	C	151	ASP	CB-CG-OD2	5.06	122.86	118.30
2	C	70	ASP	CB-CG-OD2	5.04	122.83	118.30
3	D	144	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	304	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	560	ASP	CB-CG-OD2	5.01	122.81	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	NAG	C1

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Mol	Chain	Res	Type	Atom
4	B	1001	NAG	C1

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	4277	0	4103	60	0
1	B	4381	0	4198	81	0
2	C	1657	0	1604	25	0
2	E	1657	0	1604	19	0
3	D	1665	0	1623	36	0
3	F	1665	0	1623	37	0
4	A	56	0	50	0	0
4	B	56	0	50	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	B	39	0	34	0	0
All	All	15481	0	14915	248	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 8.

All (248) 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)
2:E:142:ARG:HG2	2:E:142:ARG:HH11	1.06	1.08
3:F:30:THR:HG21	3:F:73:ARG:NH2	1.76	1.00
3:F:30:THR:HG21	3:F:73:ARG:HH21	1.23	0.99
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.50	0.91
2:E:142:ARG:HG2	2:E:142:ARG:NH1	1.82	0.90
1:A:447:HIS:HD2	1:A:448:HIS:HD2	1.19	0.89
1:B:528:LEU:HB2	1:B:529:PRO:HD3	1.56	0.86
1:B:447:HIS:HD2	1:B:448:HIS:HD2	1.25	0.84
1:A:362:ASP:OD2	1:A:364:ALA:HB3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:VAL:HG12	1:B:438:GLU:HB3	1.65	0.76
1:A:447:HIS:HD2	1:A:448:HIS:CD2	2.04	0.75
3:F:87:THR:HG23	3:F:110:THR:HA	1.67	0.74
3:D:34:MET:HB2	3:D:78:LEU:HD21	1.70	0.74
1:A:408:VAL:HG12	1:A:438:GLU:HB3	1.68	0.73
3:F:95:ASN:OD1	3:F:99:SER:O	2.06	0.73
1:B:447:HIS:HD2	1:B:448:HIS:CD2	2.05	0.73
1:A:50:SER:O	1:A:53:GLN:HG2	1.89	0.72
3:D:97:GLY:C	3:D:99:SER:H	1.93	0.72
1:B:362:ASP:OD2	1:B:364:ALA:HB3	1.89	0.72
1:B:50:SER:O	1:B:53:GLN:HG2	1.90	0.71
1:A:528:LEU:CB	1:A:529:PRO:HD3	2.18	0.71
1:A:447:HIS:CD2	1:A:448:HIS:HD2	2.08	0.69
3:F:30:THR:CG2	3:F:73:ARG:HH21	2.02	0.69
3:F:12:VAL:HG21	3:F:82(C):LEU:HD13	1.74	0.69
1:A:186:SER:HB3	1:A:189:ASP:OD1	1.93	0.69
1:B:347:LYS:HE2	1:B:349:PHE:CZ	2.29	0.68
2:E:142:ARG:CG	2:E:142:ARG:HH11	1.95	0.68
1:B:186:SER:HB3	1:B:189:ASP:OD1	1.94	0.67
2:E:136:LEU:HD11	2:E:196:VAL:HG21	1.75	0.67
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.76	0.67
1:A:338:ASN:O	1:A:341:GLU:HB2	1.95	0.67
1:A:144:THR:HG23	1:A:181:ARG:HA	1.76	0.66
1:B:338:ASN:O	1:B:341:GLU:HB2	1.95	0.66
1:A:227:HIS:CD2	1:A:241:ILE:HG23	2.31	0.66
1:B:144:THR:HG23	1:B:181:ARG:HA	1.79	0.65
1:B:415:HIS:CE1	1:B:416:ASN:ND2	2.65	0.64
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.34	0.63
3:F:69:LEU:HD22	3:F:80:LEU:HD13	1.82	0.62
1:A:332:ARG:CB	1:A:332:ARG:HH11	2.13	0.62
1:B:432:GLY:HA2	1:B:505:GLN:OE1	2.00	0.62
3:D:120:SER:HB2	3:D:122:PHE:CZ	2.34	0.62
2:C:35:TRP:HB2	2:C:48:ILE:HB	1.82	0.62
2:C:135:LEU:HD22	3:D:181:VAL:HG11	1.81	0.61
1:A:12:ARG:NH1	1:A:416:ASN:OD1	2.33	0.61
3:F:22:CYS:HB3	3:F:78:LEU:HD13	1.81	0.61
1:B:447:HIS:CD2	1:B:448:HIS:HD2	2.12	0.61
1:B:514:ARG:NH1	1:B:531:GLU:OE2	2.34	0.61
3:F:116:THR:HG22	3:F:147:PRO:HD3	1.82	0.61
1:A:57:GLU:HG3	1:A:79:ILE:HG23	1.81	0.61
2:C:94:TYR:CD2	2:C:95:PRO:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:161:GLU:HG2	2:C:175:LEU:HD21	1.83	0.60
3:D:51:VAL:CG1	3:D:78:LEU:HD23	2.32	0.60
3:D:119:PRO:HB3	3:D:145:TYR:HB3	1.82	0.60
1:A:471:LEU:HD13	1:A:473:HIS:CD2	2.36	0.60
1:B:253:ASN:O	1:B:254:THR:HB	2.01	0.60
1:B:215:HIS:CD2	1:B:227:HIS:HB3	2.37	0.59
3:D:12:VAL:HG21	3:D:82(C):LEU:HD13	1.83	0.59
1:B:471:LEU:HD13	1:B:473:HIS:CD2	2.37	0.59
1:B:81:ARG:HG2	1:B:127:LEU:HD12	1.84	0.59
1:A:332:ARG:HB2	1:A:332:ARG:HH11	1.67	0.59
1:A:81:ARG:HG2	1:A:127:LEU:HD12	1.85	0.59
1:B:227:HIS:CD2	1:B:241:ILE:HG23	2.38	0.58
1:A:71:GLN:HE22	1:A:75:GLN:HE22	1.50	0.58
1:A:528:LEU:HB2	1:A:529:PRO:CD	2.29	0.58
1:A:351:SER:HB3	1:A:387:TYR:H	1.68	0.58
3:F:33:THR:HG22	3:F:52:ASN:HA	1.84	0.58
1:A:253:ASN:O	1:A:254:THR:HB	2.03	0.57
1:A:415:HIS:CE1	1:A:416:ASN:ND2	2.73	0.56
3:F:52(A):PRO:HA	3:F:71:VAL:HG21	1.87	0.56
1:B:332:ARG:HH11	1:B:332:ARG:CB	2.18	0.56
3:F:97:GLY:C	3:F:99:SER:H	2.09	0.56
3:D:97:GLY:C	3:D:99:SER:N	2.59	0.56
1:B:57:GLU:HG3	1:B:79:ILE:HG23	1.88	0.56
1:A:144:THR:CG2	1:A:182:CYS:H	2.17	0.56
3:F:59:TYR:CE1	3:F:64:LYS:HB2	2.41	0.56
1:B:290:THR:HG21	3:F:31:ASP:OD2	2.06	0.56
2:C:149:LYS:HD3	2:C:195:GLU:HG3	1.87	0.55
3:F:35:ASP:OD2	3:F:50:ASP:HB2	2.07	0.54
2:C:79:GLN:HG3	2:C:80:PRO:HD2	1.89	0.54
1:A:194:THR:HG22	1:A:204:ARG:HD3	1.89	0.54
2:C:11:LEU:HD21	2:C:19:VAL:HG13	1.89	0.54
1:B:73:PRO:HA	1:B:75:GLN:HE22	1.73	0.54
1:A:492:LEU:O	1:A:510:SER:HB3	2.07	0.54
3:F:38:ARG:NE	3:F:46:GLU:OE1	2.41	0.54
1:A:446:ILE:HD12	1:A:471:LEU:HD21	1.90	0.54
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.89	0.54
2:C:79:GLN:HA	2:C:79:GLN:HE21	1.73	0.53
1:B:144:THR:CG2	1:B:182:CYS:H	2.21	0.53
3:D:119:PRO:HB2	3:D:142:VAL:HG12	1.90	0.53
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.44	0.53
1:B:71:GLN:HE22	1:B:75:GLN:HE22	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:LEU:HD23	2:C:55:TYR:CD1	2.44	0.53
2:C:148:TRP:HE1	2:C:177:SER:HB3	1.73	0.53
2:E:54:ARG:HD3	2:E:62:PHE:O	2.09	0.52
1:A:290:THR:HG21	3:D:31:ASP:OD2	2.10	0.52
3:D:173:SER:HB2	3:D:175:LEU:HD12	1.92	0.52
1:A:404:GLN:HG2	1:A:434:ARG:NH1	2.25	0.52
3:D:166:PHE:HB2	3:D:179:SER:O	2.09	0.52
1:B:351:SER:HB3	1:B:387:TYR:H	1.75	0.51
3:F:165:THR:HG23	3:F:180:SER:HB2	1.92	0.51
1:B:385:THR:HA	1:B:410:ARG:HB2	1.93	0.50
1:B:71:GLN:CD	1:B:119:GLN:HE21	2.15	0.50
3:D:123:PRO:HD3	3:D:209:LYS:HG2	1.93	0.50
2:E:136:LEU:HD11	2:E:196:VAL:CG2	2.41	0.50
1:A:7:THR:HG22	1:A:418:ALA:HB2	1.94	0.50
3:D:66:ARG:NH1	3:D:86:ASP:OD2	2.44	0.50
1:B:404:GLN:HG2	1:B:434:ARG:NH1	2.26	0.50
1:A:333:ALA:HB2	1:A:355:LEU:HD22	1.94	0.50
1:B:490:HIS:CE1	1:B:492:LEU:HD22	2.46	0.50
3:F:39:GLN:HG3	3:F:44:GLY:O	2.12	0.50
1:B:286:VAL:HG22	3:F:33:THR:HG23	1.94	0.50
1:A:466:ASN:HB2	1:A:467:PRO:HD2	1.94	0.49
2:E:135:LEU:CD1	3:F:181:VAL:HG21	2.42	0.49
1:A:528:LEU:CB	1:A:529:PRO:CD	2.89	0.49
1:B:523:ARG:HG2	1:B:527:GLY:HA3	1.93	0.49
2:E:146:VAL:HG21	2:E:175:LEU:HD22	1.95	0.49
1:B:401:SER:O	1:B:404:GLN:HB2	2.12	0.49
1:B:466:ASN:HB2	1:B:467:PRO:HD2	1.95	0.49
3:D:97:GLY:O	3:D:99:SER:N	2.46	0.49
1:B:446:ILE:HD12	1:B:471:LEU:HD21	1.95	0.48
3:F:120:SER:HB3	3:F:122:PHE:CZ	2.48	0.48
1:B:528:LEU:HB2	1:B:529:PRO:CD	2.38	0.48
3:D:200:HIS:HB3	3:D:203:SER:HB3	1.96	0.48
1:A:284:THR:CG2	1:A:286:VAL:H	2.26	0.48
1:B:446:ILE:HG22	1:B:476:ASN:HD21	1.77	0.48
1:A:73:PRO:HA	1:A:75:GLN:HE22	1.79	0.48
1:B:286:VAL:CG2	3:F:33:THR:HG23	2.44	0.48
3:D:200:HIS:CE1	3:D:202:PRO:HD2	2.49	0.48
1:A:446:ILE:HG22	1:A:476:ASN:HD21	1.78	0.48
1:B:284:THR:CG2	1:B:286:VAL:H	2.27	0.48
3:F:146:PHE:HB2	3:F:175:LEU:HD23	1.96	0.47
1:B:332:ARG:HH11	1:B:332:ARG:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:97:GLY:C	3:F:99:SER:N	2.67	0.47
1:A:251:THR:O	1:A:259:SER:HA	2.14	0.47
2:C:54:ARG:NH1	2:C:60:SER:HA	2.28	0.47
3:F:173:SER:HB2	3:F:175:LEU:HD12	1.96	0.47
1:A:385:THR:HA	1:A:410:ARG:HB2	1.96	0.47
3:F:71:VAL:HG12	3:F:78:LEU:HB3	1.97	0.47
1:A:401:SER:O	1:A:404:GLN:HB2	2.14	0.47
2:E:133:VAL:HG22	2:E:178:THR:HG23	1.97	0.47
3:D:139:GLY:HA2	3:D:154:TRP:CZ2	2.49	0.47
2:E:198:HIS:CD2	2:E:200:GLY:H	2.32	0.47
2:E:136:LEU:HB2	2:E:175:LEU:HB3	1.97	0.47
1:A:285:ASP:OD2	1:A:311:LYS:HE2	2.15	0.47
3:D:35:ASP:OD1	3:D:50:ASP:OD1	2.32	0.46
3:D:11:LEU:HD13	3:D:146:PHE:HE1	1.81	0.46
1:B:571:PRO:HA	1:B:572:PRO:HA	1.71	0.46
2:C:175:LEU:HD23	2:C:176:SER:N	2.29	0.46
1:A:96:ASP:HA	1:A:135:ARG:O	2.15	0.46
1:B:251:THR:O	1:B:259:SER:HA	2.15	0.46
3:D:12:VAL:HG23	3:D:111:VAL:HG22	1.96	0.46
3:D:87:THR:HG23	3:D:110:THR:HA	1.98	0.46
1:B:333:ALA:HB2	1:B:355:LEU:HD22	1.98	0.46
1:B:96:ASP:HA	1:B:135:ARG:O	2.15	0.46
3:D:52(A):PRO:HA	3:D:71:VAL:HG21	1.97	0.46
1:A:2:GLN:HG3	1:A:3:VAL:HG23	1.98	0.46
1:B:407:GLN:HB3	1:B:437:ARG:HE	1.80	0.46
2:E:4:MET:HE2	2:E:90:GLN:HB3	1.97	0.45
1:B:516:GLN:HE21	1:B:516:GLN:HA	1.82	0.45
2:E:20:THR:HG23	2:E:74:THR:HG23	1.97	0.45
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.89	0.45
2:C:118:PHE:HA	2:C:119:PRO:HD3	1.84	0.45
1:A:22:ASP:O	1:A:26:HIS:HD2	1.99	0.45
2:C:19:VAL:HG21	2:C:78:LEU:HD22	1.99	0.45
1:A:284:THR:HG23	1:A:286:VAL:H	1.82	0.45
1:B:415:HIS:CE1	1:B:416:ASN:HD22	2.35	0.45
1:B:290:THR:HG21	3:F:31:ASP:OD1	2.17	0.45
1:A:164:THR:OG1	1:B:160:THR:HB	2.16	0.45
1:A:351:SER:HB3	1:A:387:TYR:O	2.16	0.45
3:F:96:LEU:HD22	3:F:101:ASP:HB3	1.98	0.45
3:D:35:ASP:OD1	3:D:95:ASN:HB2	2.15	0.45
1:B:10:LYS:HB3	1:B:11:LEU:H	1.61	0.45
3:F:146:PHE:HA	3:F:147:PRO:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:HD23	1:B:518:CYS:O	2.17	0.44
2:E:116:PHE:HB2	2:E:135:LEU:HB3	2.00	0.44
2:C:2:ILE:HG12	2:C:2:ILE:H	1.67	0.44
2:E:135:LEU:HD11	3:F:181:VAL:HG21	2.00	0.44
3:D:201:LYS:HB2	3:D:202:PRO:HD3	1.99	0.44
3:D:148:GLU:HA	3:D:149:PRO:HA	1.66	0.44
2:C:36:TYR:HE2	2:C:89:GLN:OE1	2.01	0.44
1:B:559:ALA:HB1	1:B:574:CYS:H	1.83	0.44
1:A:355:LEU:O	1:A:358:SER:HB2	2.18	0.44
1:B:80:VAL:HG13	1:B:126:ILE:HG12	1.99	0.44
3:F:96:LEU:HD12	3:F:96:LEU:HA	1.75	0.44
3:F:15:GLY:HA2	3:F:82(B):SER:HA	2.00	0.44
1:B:490:HIS:HE1	1:B:492:LEU:HD22	1.81	0.43
1:B:570:ASP:HA	1:B:571:PRO:HD3	1.90	0.43
3:D:119:PRO:CB	3:D:145:TYR:HB3	2.47	0.43
1:B:548:GLN:HG3	1:B:563:VAL:HG11	1.99	0.43
3:F:145:TYR:CE2	3:F:150:VAL:HG13	2.54	0.43
3:D:52:ASN:HA	3:D:52(A):PRO:HD3	1.83	0.43
1:B:487:LEU:HA	1:B:487:LEU:HD23	1.91	0.43
2:C:193:ALA:HB1	2:C:206:THR:CG2	2.49	0.43
1:A:422:THR:HA	1:A:445:LEU:O	2.19	0.43
3:D:146:PHE:HA	3:D:147:PRO:HA	1.70	0.43
1:B:194:THR:HG22	1:B:204:ARG:HD3	2.01	0.43
3:D:3:GLN:HG3	3:D:25:SER:OG	2.19	0.42
1:A:80:VAL:HG13	1:A:126:ILE:HG12	2.01	0.42
2:C:106:ILE:HG23	2:C:166:GLN:HE21	1.83	0.42
1:B:315:PRO:HD3	2:E:53:TYR:CE1	2.54	0.42
1:B:494:ALA:C	1:B:496:GLY:N	2.72	0.42
1:A:407:GLN:HB3	1:A:437:ARG:HE	1.84	0.42
3:F:121:VAL:HG22	3:F:142:VAL:HG13	2.00	0.42
1:A:9:MET:O	1:A:12:ARG:HB2	2.20	0.42
2:C:52:SER:HA	2:C:64:GLY:O	2.20	0.42
3:F:69:LEU:CD2	3:F:80:LEU:HD13	2.48	0.42
3:D:200:HIS:ND1	3:D:202:PRO:HD2	2.35	0.42
3:D:85:GLU:H	3:D:85:GLU:HG3	1.69	0.42
2:E:93:ILE:HD13	2:E:93:ILE:HA	1.87	0.42
1:B:125:GLU:OE1	1:B:219:ALA:O	2.38	0.42
1:A:146:LEU:HD11	1:A:196:THR:HG21	2.01	0.42
1:B:351:SER:HB3	1:B:387:TYR:O	2.19	0.42
2:C:107:LYS:HA	2:C:140:TYR:OH	2.19	0.42
3:D:67:PHE:HB3	3:D:80:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:ASN:OD1	3:D:98:PRO:HA	2.20	0.41
2:E:79:GLN:NE2	2:E:79:GLN:HA	2.35	0.41
1:B:410:ARG:HD3	1:B:412:ARG:NH2	2.34	0.41
1:B:111:SER:N	1:B:112:PRO:HD2	2.35	0.41
1:A:111:SER:N	1:A:112:PRO:HD2	2.36	0.41
1:A:134:GLN:HA	1:A:163:ASP:HB3	2.02	0.41
1:B:146:LEU:HD12	1:B:149:ASP:HB2	2.01	0.41
2:C:79:GLN:HA	2:C:79:GLN:NE2	2.36	0.41
1:B:17:PRO:HD2	1:B:18:GLU:OE1	2.21	0.41
1:B:16:SER:HA	1:B:17:PRO:HD3	1.89	0.41
3:F:97:GLY:O	3:F:99:SER:N	2.54	0.41
2:C:37:GLN:HG3	2:C:86:TYR:CE2	2.55	0.41
1:B:146:LEU:HD11	1:B:196:THR:HG21	2.02	0.41
2:C:203:SER:HA	2:C:204:PRO:HD2	1.93	0.41
1:B:284:THR:HG23	1:B:286:VAL:H	1.86	0.41
1:A:146:LEU:HD12	1:A:149:ASP:HB2	2.02	0.41
3:D:6:GLU:HG3	3:D:92:CYS:HB3	2.03	0.41
1:A:234:LEU:HD13	1:A:235:HIS:CE1	2.56	0.41
1:B:134:GLN:HA	1:B:163:ASP:HB3	2.02	0.41
3:D:35:ASP:OD2	3:D:50:ASP:HB2	2.21	0.41
1:A:319:VAL:HG13	1:A:349:PHE:CD1	2.56	0.41
1:B:559:ALA:HB3	1:B:573:PHE:HD2	1.85	0.41
1:A:71:GLN:CD	1:A:119:GLN:HE21	2.24	0.41
1:B:72:VAL:HA	1:B:73:PRO:HD3	1.91	0.41
1:B:542:HIS:HD2	1:B:544:GLU:HB2	1.86	0.41
1:B:43:LEU:HD13	1:B:49:LEU:HD21	2.03	0.41
1:B:262:ASN:HA	1:B:263:PRO:HD2	1.91	0.40
2:C:89:GLN:HB2	2:C:98:PHE:CD2	2.55	0.40
1:B:548:GLN:HG3	1:B:563:VAL:CG1	2.52	0.40
1:B:24:LEU:HD23	1:B:43:LEU:HD21	2.03	0.40
1:B:362:ASP:HA	1:B:363:PRO:HD2	1.93	0.40
3:F:59:TYR:HE1	3:F:64:LYS:HB2	1.84	0.40
1:B:285:ASP:OD2	1:B:311:LYS:HE2	2.21	0.40
1:B:546:GLN:HB2	1:B:566:ALA:HA	2.02	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	551/624 (88%)	503 (91%)	41 (7%)	7 (1%)	15	56
1	B	564/624 (90%)	513 (91%)	43 (8%)	8 (1%)	14	54
2	C	212/214 (99%)	185 (87%)	23 (11%)	4 (2%)	10	48
2	E	212/214 (99%)	192 (91%)	18 (8%)	2 (1%)	21	64
3	D	220/226 (97%)	195 (89%)	22 (10%)	3 (1%)	14	54
3	F	220/226 (97%)	197 (90%)	19 (9%)	4 (2%)	11	49
All	All	1979/2128 (93%)	1785 (90%)	166 (8%)	28 (1%)	14	54

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	A	366	ASN
1	A	404	GLN
1	B	364	ALA
1	B	366	ASN
1	B	404	GLN
1	B	576	ALA
2	E	152	ASN
1	A	363	PRO
1	B	363	PRO
2	C	30	SER
2	E	30	SER
1	A	461	ASP
1	B	313	SER
1	B	495	ARG
2	C	151	ASP
1	A	313	SER
2	C	135	LEU
3	F	96	LEU
3	F	134	GLY

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Mol	Chain	Res	Type
3	F	156	SER
3	D	96	LEU
3	F	18	LEU
2	C	199	GLN
1	A	305	GLY
1	B	305	GLY
3	D	157	GLY
3	D	147	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	478/538 (89%)	401 (84%)	77 (16%)	3 14
1	B	489/538 (91%)	414 (85%)	75 (15%)	3 17
2	C	188/188 (100%)	141 (75%)	47 (25%)	1 3
2	E	188/188 (100%)	149 (79%)	39 (21%)	1 7
3	D	187/191 (98%)	142 (76%)	45 (24%)	1 3
3	F	187/191 (98%)	143 (76%)	44 (24%)	1 4
All	All	1717/1834 (94%)	1390 (81%)	327 (19%)	2 9

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	THR
1	A	16	SER
1	A	21	LEU
1	A	24	LEU
1	A	27	LEU
1	A	29	GLN
1	A	31	CYS
1	A	32	GLN
1	A	45	THR

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Mol	Chain	Res	Type
1	A	46	ASN
1	A	50	SER
1	A	53	GLN
1	A	59	GLN
1	A	68	GLN
1	A	71	GLN
1	A	72	VAL
1	A	77	LEU
1	A	78	ARG
1	A	80	VAL
1	A	101	LEU
1	A	116	ARG
1	A	144	THR
1	A	146	LEU
1	A	159	LEU
1	A	160	THR
1	A	176	MET
1	A	181	ARG
1	A	188	GLU
1	A	191	GLN
1	A	206	LYS
1	A	211	THR
1	A	216	GLU
1	A	234	LEU
1	A	239	SER
1	A	241	ILE
1	A	250	VAL
1	A	254	THR
1	A	258	GLU
1	A	274	VAL
1	A	284	THR
1	A	286	VAL
1	A	298	GLN
1	A	306	THR
1	A	314	LYS
1	A	318	ARG
1	A	332	ARG
1	A	339	ILE
1	A	346	LYS
1	A	351	SER
1	A	357	GLU
1	A	360	ASP

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Mol	Chain	Res	Type
1	A	365	SER
1	A	367	THR
1	A	380	THR
1	A	410	ARG
1	A	429	SER
1	A	434	ARG
1	A	437	ARG
1	A	450	THR
1	A	461	ASP
1	A	471	LEU
1	A	477	ARG
1	A	483	VAL
1	A	495	ARG
1	A	504	THR
1	A	510	SER
1	A	518	CYS
1	A	524	VAL
1	A	525	LEU
1	A	526	GLN
1	A	536	ARG
1	A	544	GLU
1	A	546	GLN
1	A	552	VAL
1	A	558	GLU
1	A	561	GLN
1	B	5	THR
1	B	7	THR
1	B	16	SER
1	B	21	LEU
1	B	24	LEU
1	B	27	LEU
1	B	29	GLN
1	B	31	CYS
1	B	32	GLN
1	B	45	THR
1	B	46	ASN
1	B	50	SER
1	B	53	GLN
1	B	59	GLN
1	B	68	GLN
1	B	71	GLN
1	B	72	VAL

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Mol	Chain	Res	Type
1	B	77	LEU
1	B	78	ARG
1	B	80	VAL
1	B	84	GLN
1	B	101	LEU
1	B	144	THR
1	B	146	LEU
1	B	159	LEU
1	B	160	THR
1	B	176	MET
1	B	188	GLU
1	B	191	GLN
1	B	206	LYS
1	B	211	THR
1	B	216	GLU
1	B	226	LYS
1	B	234	LEU
1	B	239	SER
1	B	241	ILE
1	B	250	VAL
1	B	251	THR
1	B	254	THR
1	B	258	GLU
1	B	274	VAL
1	B	284	THR
1	B	286	VAL
1	B	298	GLN
1	B	306	THR
1	B	314	LYS
1	B	318	ARG
1	B	332	ARG
1	B	339	ILE
1	B	346	LYS
1	B	351	SER
1	B	357	GLU
1	B	360	ASP
1	B	365	SER
1	B	367	THR
1	B	380	THR
1	B	410	ARG
1	B	429	SER
1	B	434	ARG

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Mol	Chain	Res	Type
1	B	437	ARG
1	B	450	THR
1	B	461	ASP
1	B	471	LEU
1	B	492	LEU
1	B	495	ARG
1	B	504	THR
1	B	509	CYS
1	B	510	SER
1	B	513	LEU
1	B	516	GLN
1	B	552	VAL
1	B	558	GLU
1	B	569	LYS
1	B	575	VAL
1	B	577	ARG
2	C	1	ASP
2	C	2	ILE
2	C	3	GLN
2	C	7	SER
2	C	9	SER
2	C	10	SER
2	C	11	LEU
2	C	12	SER
2	C	22	THR
2	C	27	GLN
2	C	50	SER
2	C	54	ARG
2	C	63	SER
2	C	67	SER
2	C	72	THR
2	C	79	GLN
2	C	93	ILE
2	C	105	GLU
2	C	106	ILE
2	C	107	LYS
2	C	110	VAL
2	C	114	SER
2	C	122	ASP
2	C	124	GLN
2	C	126	LYS
2	C	129	THR

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Mol	Chain	Res	Type
2	C	133	VAL
2	C	135	LEU
2	C	142	ARG
2	C	147	GLN
2	C	156	SER
2	C	158	ASN
2	C	159	SER
2	C	168	SER
2	C	169	LYS
2	C	177	SER
2	C	179	LEU
2	C	181	LEU
2	C	183	LYS
2	C	199	GLN
2	C	202	SER
2	C	205	VAL
2	C	207	LYS
2	C	209	PHE
2	C	210	ASN
2	C	211	ARG
2	C	214	CYS
3	D	11	LEU
3	D	19	ARG
3	D	33	THR
3	D	62	ARG
3	D	64	LYS
3	D	68	THR
3	D	70	SER
3	D	71	VAL
3	D	74	SER
3	D	75	LYS
3	D	82	MET
3	D	82(B)	SER
3	D	83	ARG
3	D	85	GLU
3	D	92	CYS
3	D	99	SER
3	D	100	PHE
3	D	108	LEU
3	D	113	SER
3	D	115	SER
3	D	116	THR

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Mol	Chain	Res	Type
3	D	117	LYS
3	D	120	SER
3	D	121	VAL
3	D	129	LYS
3	D	130	SER
3	D	131	THR
3	D	135	THR
3	D	141	LEU
3	D	142	VAL
3	D	143	LYS
3	D	152	VAL
3	D	156	SER
3	D	166	PHE
3	D	173	SER
3	D	183	THR
3	D	189	LEU
3	D	192	GLN
3	D	193	THR
3	D	195	ILE
3	D	199	ASN
3	D	206	LYS
3	D	209	LYS
3	D	214	LYS
3	D	215	SER
2	E	1	ASP
2	E	2	ILE
2	E	3	GLN
2	E	5	THR
2	E	9	SER
2	E	11	LEU
2	E	14	SER
2	E	20	THR
2	E	31	ILE
2	E	54	ARG
2	E	70	ASP
2	E	72	THR
2	E	79	GLN
2	E	93	ILE
2	E	109	THR
2	E	110	VAL
2	E	115	VAL
2	E	123	GLU

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Mol	Chain	Res	Type
2	E	124	GLN
2	E	129	THR
2	E	132	VAL
2	E	142	ARG
2	E	145	LYS
2	E	154	LEU
2	E	155	GLN
2	E	159	SER
2	E	163	VAL
2	E	166	GLN
2	E	168	SER
2	E	171	SER
2	E	182	SER
2	E	185	ASP
2	E	188	LYS
2	E	190	LYS
2	E	191	VAL
2	E	197	THR
2	E	199	GLN
2	E	213	GLU
2	E	214	CYS
3	F	1	GLU
3	F	7	SER
3	F	11	LEU
3	F	12	VAL
3	F	19	ARG
3	F	21	SER
3	F	30	THR
3	F	62	ARG
3	F	64	LYS
3	F	69	LEU
3	F	70	SER
3	F	74	SER
3	F	78	LEU
3	F	82	MET
3	F	82(A)	ASN
3	F	82(B)	SER
3	F	83	ARG
3	F	92	CYS
3	F	99	SER
3	F	108	LEU
3	F	115	SER

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Mol	Chain	Res	Type
3	F	117	LYS
3	F	129	LYS
3	F	132	SER
3	F	135	THR
3	F	151	THR
3	F	153	SER
3	F	163	VAL
3	F	169	VAL
3	F	170	LEU
3	F	173	SER
3	F	184	VAL
3	F	189	LEU
3	F	191	THR
3	F	197	ASN
3	F	199	ASN
3	F	201	LYS
3	F	204	ASN
3	F	205	THR
3	F	206	LYS
3	F	209	LYS
3	F	210	LYS
3	F	212	GLU
3	F	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	71	GLN
1	A	75	GLN
1	A	119	GLN
1	A	138	GLN
1	A	156	GLN
1	A	245	HIS
1	A	366	ASN
1	A	415	HIS
1	A	424	GLN
1	A	447	HIS
1	A	448	HIS
1	A	473	HIS
1	A	516	GLN
1	B	26	HIS

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	119	GLN
1	B	138	GLN
1	B	156	GLN
1	B	245	HIS
1	B	366	ASN
1	B	415	HIS
1	B	416	ASN
1	B	447	HIS
1	B	448	HIS
1	B	473	HIS
1	B	497	HIS
1	B	516	GLN
1	B	537	HIS
1	B	542	HIS
1	B	546	GLN
2	C	3	GLN
2	C	79	GLN
2	C	147	GLN
2	C	160	GLN
2	C	166	GLN
3	D	76	ASN
2	E	79	GLN
2	E	155	GLN
2	E	198	HIS
2	E	210	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

11 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	$\#\|Z\| > 2$
4	NAG	A	1001	1,4	14,14,15	1.27	1 (7%)	15,19,21	2.59	4 (26%)
4	NAG	A	1002	4	14,14,15	0.76	0	15,19,21	1.48	1 (6%)
4	NAG	A	1003	1,4	14,14,15	0.64	0	15,19,21	1.13	1 (6%)
4	NAG	A	1004	4	14,14,15	0.55	0	15,19,21	1.43	2 (13%)
4	NAG	B	1001	1,4	14,14,15	1.15	1 (7%)	15,19,21	2.47	4 (26%)
4	NAG	B	1002	4	14,14,15	0.69	0	15,19,21	1.33	2 (13%)
6	NAG	B	1003	1,6	14,14,15	0.60	0	15,19,21	1.14	1 (6%)
6	NAG	B	1004	6	14,14,15	0.64	0	15,19,21	1.39	2 (13%)
6	BMA	B	1005	6	11,11,12	0.60	0	14,15,17	1.08	1 (7%)
4	NAG	B	1007	1,4	14,14,15	0.52	0	15,19,21	1.60	1 (6%)
4	NAG	B	1008	4	14,14,15	0.49	0	15,19,21	0.73	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
4	NAG	A	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1002	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1003	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1004	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	1002	4	-	0/6/23/26	0/1/1/1
6	NAG	B	1003	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1004	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1005	6	-	0/2/19/22	0/1/1/1
4	NAG	B	1007	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	4	-	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)
4	B	1001	NAG	C1-C2	2.56	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAG	C1-C2	2.74	1.56	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	NAG	C3-C4-C5	-3.67	103.80	110.20
4	B	1001	NAG	C3-C4-C5	-3.24	104.55	110.20
4	A	1001	NAG	O7-C7-C8	-2.02	118.35	122.06
4	B	1002	NAG	O7-C7-N2	2.02	125.98	121.86
4	B	1001	NAG	C3-C2-N2	2.07	115.52	110.56
4	A	1003	NAG	C1-O5-C5	2.48	115.40	112.25
4	A	1004	NAG	C3-C4-C5	2.50	114.56	110.20
6	B	1005	BMA	O5-C5-C6	2.69	113.18	107.35
6	B	1004	NAG	C3-C4-C5	2.92	115.29	110.20
6	B	1003	NAG	C2-N2-C7	3.10	127.02	123.04
4	B	1002	NAG	C1-O5-C5	3.63	116.86	112.25
6	B	1004	NAG	C4-C3-C2	3.64	116.88	111.23
4	A	1004	NAG	C4-C3-C2	3.95	117.37	111.23
4	B	1001	NAG	O4-C4-C3	4.18	119.74	110.34
4	A	1002	NAG	C1-O5-C5	4.30	117.70	112.25
4	A	1001	NAG	O4-C4-C3	4.53	120.53	110.34
4	B	1007	NAG	C1-O5-C5	4.95	118.53	112.25
4	B	1001	NAG	C2-N2-C7	6.29	131.12	123.04
4	A	1001	NAG	C2-N2-C7	6.69	131.63	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1001	NAG	C1
4	A	1001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

2 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	$\#\|Z\| > 2$
5	NAG	A	1006	1	14,14,15	0.85	0	15,19,21	1.86	2 (13%)
5	NAG	B	1006	1	14,14,15	0.61	0	15,19,21	1.22	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
5	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1006	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1006	NAG	C1-O5-C5	2.36	115.25	112.25
5	B	1006	NAG	C2-N2-C7	3.18	127.13	123.04
5	A	1006	NAG	C3-C4-C5	3.56	116.41	110.20
5	A	1006	NAG	C1-O5-C5	5.30	118.98	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	555/624 (88%)	-0.21	20 (3%) 46 37	3, 10, 13, 25	0
1	B	568/624 (91%)	-0.17	12 (2%) 67 57	3, 10, 13, 24	0
2	C	214/214 (100%)	0.50	34 (15%) 3 2	2, 10, 17, 26	0
2	E	214/214 (100%)	-0.32	2 (0%) 85 80	2, 10, 18, 24	0
3	D	222/226 (98%)	0.51	27 (12%) 5 4	2, 10, 17, 32	0
3	F	222/226 (98%)	-0.09	9 (4%) 41 31	2, 11, 19, 29	0
All	All	1995/2128 (93%)	-0.04	104 (5%) 31 22	2, 10, 16, 32	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	128	SER	16.8
3	F	130	SER	9.8
3	D	130	SER	8.0
2	C	193	ALA	7.5
2	C	130	ALA	7.4
3	D	125	ALA	7.1
2	C	119	PRO	7.0
2	C	212	GLY	6.2
1	A	544	GLU	6.2
2	C	208	SER	6.2
2	C	129	THR	6.1
2	E	214	CYS	5.2
2	C	187	GLU	5.2
3	D	127	SER	5.2
3	D	216	CYS	4.8
2	C	196	VAL	4.8
3	D	129	LYS	4.7
2	C	131	SER	4.6
2	C	120	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	546	GLN	4.5
2	C	214	CYS	4.5
1	A	545	CYS	4.2
2	C	194	CYS	4.2
3	D	214	LYS	4.0
2	C	186	TYR	3.9
1	A	547	PRO	3.9
2	C	192	TYR	3.8
3	D	215	SER	3.7
2	E	212	GLY	3.7
2	C	211	ARG	3.7
1	A	543	PRO	3.6
2	C	181	LEU	3.6
3	D	139	GLY	3.5
3	D	140	CYS	3.5
3	D	199	ASN	3.4
3	F	207	VAL	3.4
1	A	562	CYS	3.3
1	B	180	SER	3.3
3	F	132	SER	3.3
3	D	206	LYS	3.2
1	B	576	ALA	3.2
2	C	180	THR	3.2
3	D	158	ALA	3.1
1	B	577	ARG	3.1
2	C	148	TRP	3.0
1	A	564	ALA	3.0
3	F	146	PHE	3.0
3	D	156	SER	3.0
3	D	185	PRO	3.0
3	D	208	ASP	3.0
1	A	563	VAL	2.9
3	D	204	ASN	2.9
3	D	184	VAL	2.9
3	D	141	LEU	2.9
3	D	179	SER	2.8
3	D	160	THR	2.8
2	C	116	PHE	2.8
2	C	122	ASP	2.7
1	A	197	VAL	2.7
2	C	188	LYS	2.6
3	D	126	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	557	PRO	2.5
1	B	572	PRO	2.5
2	C	121	SER	2.5
1	A	513	LEU	2.5
1	B	303	GLU	2.5
2	C	178	THR	2.5
1	A	542	HIS	2.5
2	C	205	VAL	2.5
2	C	158	ASN	2.4
3	F	117	LYS	2.4
1	B	574	CYS	2.4
3	F	118	GLY	2.4
3	F	216	CYS	2.4
2	C	118	PHE	2.4
1	A	180	SER	2.4
1	A	1	THR	2.3
1	A	555	PHE	2.3
1	B	318	ARG	2.3
2	C	213	GLU	2.3
1	B	540	PRO	2.3
1	A	559	ALA	2.2
3	D	187	SER	2.2
1	B	566	ALA	2.2
3	F	131	THR	2.2
2	C	117	ILE	2.2
3	D	121	VAL	2.2
2	C	132	VAL	2.2
1	A	541	CYS	2.2
1	A	536	ARG	2.2
3	F	119	PRO	2.2
1	A	512	PHE	2.2
1	A	561	GLN	2.2
2	C	149	LYS	2.1
3	D	202	PRO	2.1
1	B	573	PHE	2.1
1	B	570	ASP	2.1
2	C	197	THR	2.1
2	C	179	LEU	2.1
3	D	157	GLY	2.1
3	D	133	GLY	2.0
2	C	209	PHE	2.0
2	C	154	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	568	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
4	NAG	A	1001	14/15	0.74	0.31	3.33	8,11,13,14	0
6	NAG	B	1003	14/15	0.88	0.23	2.27	8,11,14,14	0
4	NAG	A	1003	14/15	0.92	0.21	1.10	8,11,14,15	0
4	NAG	B	1001	14/15	0.82	0.21	0.89	8,11,13,14	0
4	NAG	A	1002	14/15	0.74	0.51	-	11,15,19,20	0
4	NAG	A	1004	14/15	0.79	0.39	-	12,15,18,19	0
4	NAG	B	1008	14/15	0.78	0.34	-	10,11,12,12	0
6	BMA	B	1005	11/12	0.74	0.22	-	19,23,28,30	0
4	NAG	B	1002	14/15	0.81	0.57	-	11,15,19,20	0
6	NAG	B	1004	14/15	0.79	0.38	-	13,15,18,19	0
4	NAG	B	1007	14/15	0.82	0.20	-	6,9,12,12	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
5	NAG	B	1006	14/15	0.89	0.43	-	54,64,67,67	0
5	NAG	A	1006	14/15	0.69	0.76	-	57,68,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.