



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:39 AM UTC

PDB ID : 8ZYF / pdb_00008zyf
Title : Crystal structure of ZW2G10 Fab in complex with omicron RBD
Authors : Yuan, H.Y.; Li, J.M.
Deposited on : 2024-06-17
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

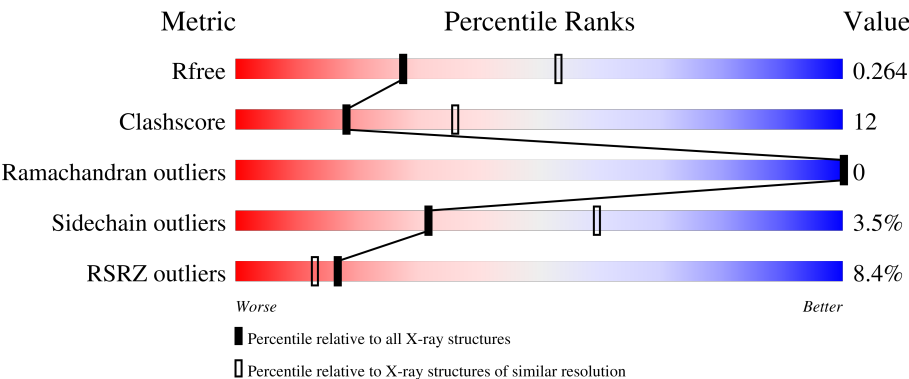
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	195	%85%14%.
1	B	195	5%85%14%.
2	C	214	10%65%29%..
2	D	214	16%70%22%5%
3	E	229	9%69%22%6%

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Mol	Chain	Length	Quality of chain
3	H	229	6% 60% 17% 22%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18204 atoms, of which 8655 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 Spike protein S1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	195	Total	C	H	N	O	S	0	0	0
			3053	1013	1485	265	282	8			
1	B	195	Total	C	H	N	O	S	0	0	0
			3053	1013	1485	265	282	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2

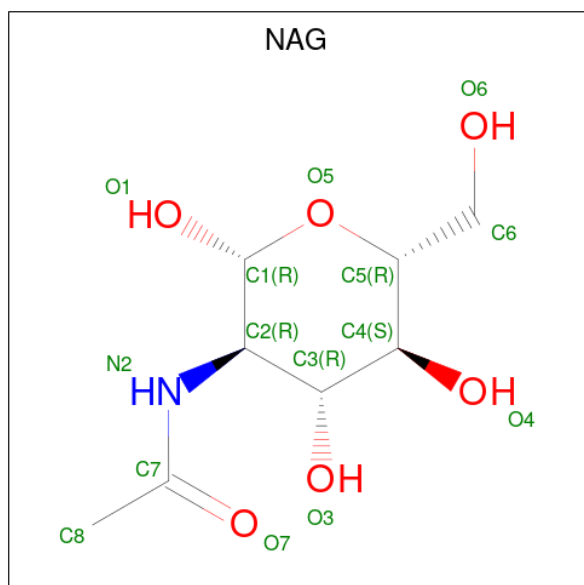
- Molecule 2 is a protein called ZW2G10 fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	203	Total	C	H	N	O	S	0	0	0
			2950	944	1438	256	308	4			
2	C	210	Total	C	H	N	O	S	0	0	0
			3047	969	1495	263	316	4			

- Molecule 3 is a protein called ZW2G10 fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	178	Total	C	H	N	O	S	0	0	0
			2655	867	1291	225	267	5			
3	E	215	Total	C	H	N	O	S	0	0	0
			3095	1033	1461	273	321	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

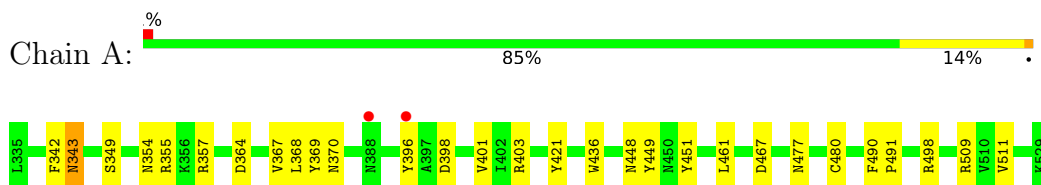
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	D	48	Total	O	0	0
			48	48		
5	H	68	Total	O	0	0
			68	68		
5	B	64	Total	O	0	0
			64	64		
5	C	38	Total	O	0	0
			38	38		
5	E	37	Total	O	0	0
			37	37		

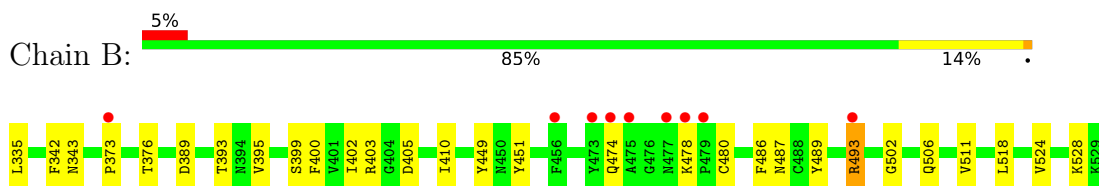
3 Residue-property plots [i](#)

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

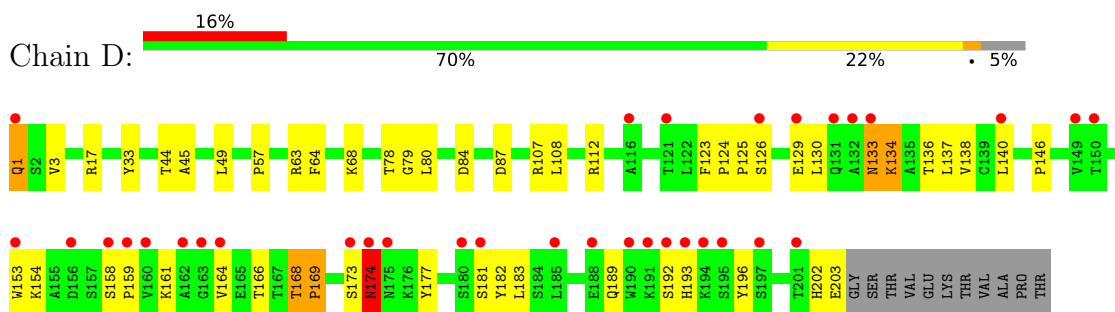
- Molecule 1: Spike protein S1



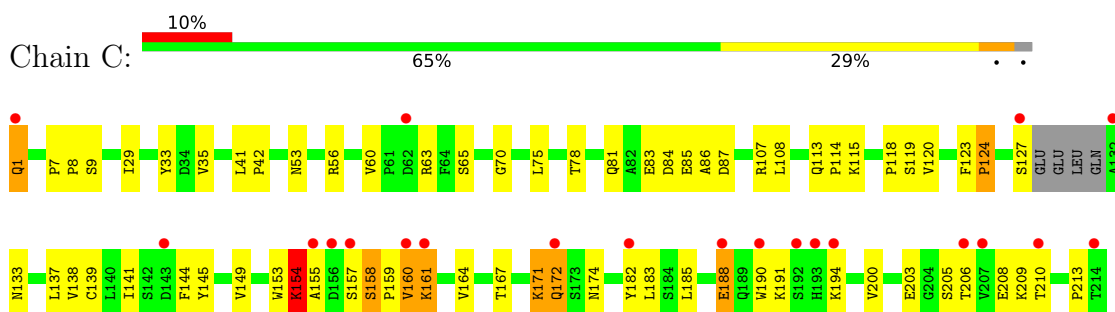
- Molecule 1: Spike protein S1



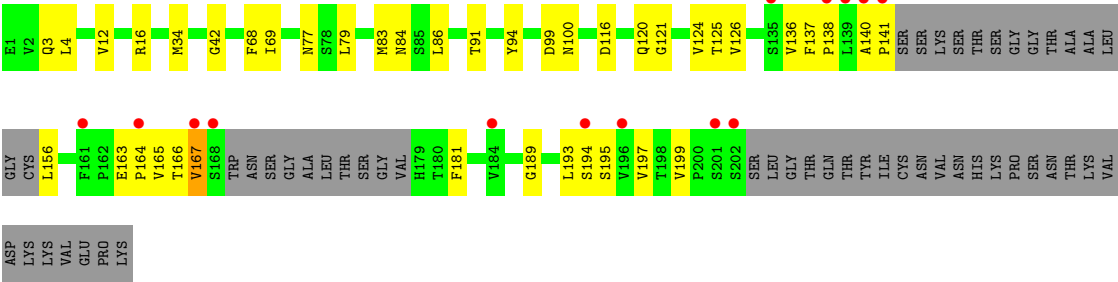
- Molecule 2: ZW2G10 fab light chain



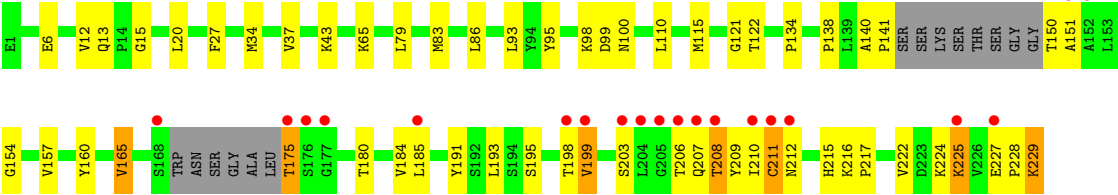
- Molecule 2: ZW2G10 fab light chain



- Molecule 3: ZW2G10 fab heavy chain



● Molecule 3: ZW2G10 fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.66Å 103.53Å 299.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.60 39.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.53-2.60) 97.9 (39.53-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, R_{free}	0.232 , 0.285 (Not available) , 0.264	Depositor DCC
R_{free} test set	2181 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18204	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/1615	0.52	2/2196 (0.1%)
1	B	0.26	0/1615	0.45	1/2196 (0.0%)
2	C	0.96	9/1589 (0.6%)	1.30	19/2170 (0.9%)
2	D	0.77	3/1549 (0.2%)	0.97	10/2115 (0.5%)
3	E	0.54	0/1673	0.81	3/2277 (0.1%)
3	H	0.32	0/1399	0.55	1/1905 (0.1%)
All	All	0.59	12/9440 (0.1%)	0.83	36/12859 (0.3%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	169	PRO	N-CA	18.34	1.68	1.47
2	C	124	PRO	N-CA	15.11	1.67	1.46
2	D	168	THR	C-N	9.97	1.45	1.33
2	C	123	PHE	C-N	9.12	1.44	1.33
2	C	118	PRO	C-O	-7.76	1.15	1.23
2	C	7	PRO	C-O	-7.56	1.16	1.24
2	C	157	SER	C-O	-6.46	1.15	1.23
2	D	177	TYR	C-O	-5.40	1.17	1.23
2	C	114	PRO	C-O	-5.22	1.17	1.23
2	C	113	GLN	C-O	-5.20	1.19	1.24
2	C	8	PRO	C-O	-5.18	1.17	1.24
2	C	9	SER	C-O	-5.08	1.18	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	123	PHE	CA-C-N	22.53	135.88	119.66
2	C	123	PHE	C-N-CA	22.53	135.88	119.66
2	D	168	THR	CA-C-N	14.66	135.62	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	168	THR	C-N-CA	14.66	135.62	119.93
2	C	124	PRO	N-CA-C	-9.25	100.68	110.58
2	C	124	PRO	CB-CA-C	8.96	119.59	111.17
2	D	169	PRO	CA-N-CD	-8.79	99.69	112.00
2	D	134	LYS	N-CA-CB	-7.86	99.01	110.87
1	A	477	ASN	CB-CA-C	-7.52	94.55	109.67
2	C	155	ALA	CA-C-N	7.25	135.40	121.54
2	C	155	ALA	C-N-CA	7.25	135.40	121.54
2	C	159	PRO	N-CA-C	-7.14	97.76	112.47
2	C	124	PRO	N-CA-CB	7.09	106.91	103.22
2	C	124	PRO	CA-N-CD	-6.86	102.40	112.00
3	E	198	THR	CB-CA-C	6.68	120.70	109.48
2	D	169	PRO	N-CA-C	-6.59	100.51	111.26
3	H	120	GLN	CA-C-O	-6.50	111.45	119.18
2	D	173	SER	CA-C-N	6.32	132.94	121.06
2	D	173	SER	C-N-CA	6.32	132.94	121.06
2	C	155	ALA	O-C-N	6.15	130.21	122.22
3	E	198	THR	CA-C-N	6.13	133.48	122.13
3	E	198	THR	C-N-CA	6.13	133.48	122.13
2	C	188	GLU	CA-C-N	5.85	128.04	120.44
2	C	188	GLU	C-N-CA	5.85	128.04	120.44
2	C	161	LYS	CB-CA-C	5.79	121.94	110.42
2	C	154	LYS	CB-CA-C	5.63	121.94	109.94
2	C	118	PRO	N-CA-C	5.57	120.98	111.68
2	D	174	ASN	N-CA-CB	-5.46	102.90	110.38
2	C	124	PRO	N-CD-CG	5.39	111.29	103.20
2	C	161	LYS	CA-C-O	-5.31	112.92	120.51
2	C	124	PRO	O-C-N	-5.30	118.66	121.15
2	D	133	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	493	ARG	CG-CD-NE	-5.20	100.57	112.00
2	D	168	THR	O-C-N	-5.08	115.18	121.64
1	A	343	ASN	CA-C-O	-5.03	114.01	119.95
2	C	8	PRO	CB-CA-C	-5.03	104.36	112.21

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	1568	1485	1507	22	0
1	B	1568	1485	1507	39	0
2	C	1552	1495	1508	52	0
2	D	1512	1438	1462	35	0
3	E	1634	1461	1582	47	0
3	H	1364	1291	1305	32	0
4	A	14	0	13	4	0
4	B	14	0	13	5	0
5	A	68	0	0	5	0
5	B	64	0	0	9	2
5	C	38	0	0	9	0
5	D	48	0	0	1	2
5	E	37	0	0	3	0
5	H	68	0	0	6	0
All	All	9549	8655	8897	218	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:HD21	4:A:601:NAG:C1	1.08	1.58
1:B:343:ASN:HD21	4:B:601:NAG:C1	1.25	1.49
1:B:478:LYS:NZ	1:B:486:PHE:HD2	1.10	1.47
2:D:169:PRO:CA	2:D:169:PRO:N	1.68	1.46
2:C:124:PRO:N	2:C:124:PRO:CA	1.67	1.43
1:B:478:LYS:NZ	1:B:486:PHE:CD2	1.92	1.34
1:B:343:ASN:ND2	4:B:601:NAG:C1	1.95	1.27
3:E:208:THR:O	5:E:301:HOH:O	1.53	1.20
3:E:150:THR:N	5:E:302:HOH:O	1.89	1.05
2:D:164:VAL:HG22	2:D:183:LEU:HD13	1.38	1.02
3:H:4:LEU:O	5:H:301:HOH:O	1.83	0.97
2:C:205:SER:O	5:C:301:HOH:O	1.82	0.96
1:B:478:LYS:NZ	1:B:486:PHE:HB3	1.81	0.95
3:E:211:CYS:SG	3:E:211:CYS:O	2.27	0.92
3:H:156:LEU:N	5:H:304:HOH:O	2.06	0.89
1:A:369:TYR:O	5:A:701:HOH:O	1.92	0.86
2:C:167:THR:CG2	3:E:184:VAL:HG12	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:LYS:HZ1	1:B:486:PHE:HD2	0.86	0.84
3:H:163:GLU:HG2	3:H:164:PRO:HA	1.61	0.83
3:E:15:GLY:O	5:E:303:HOH:O	1.96	0.83
1:B:335:LEU:N	5:B:704:HOH:O	2.11	0.81
2:C:81:GLN:OE1	5:C:302:HOH:O	1.98	0.80
3:E:225:LYS:H	3:E:225:LYS:HD2	1.47	0.80
2:C:124:PRO:O	5:C:303:HOH:O	2.00	0.79
1:B:478:LYS:CE	1:B:486:PHE:HD2	1.95	0.79
3:E:138:PRO:HG3	3:E:224:LYS:CG	2.13	0.77
1:B:478:LYS:NZ	1:B:486:PHE:CG	2.53	0.77
3:H:167:VAL:HG11	3:H:195:SER:CB	2.15	0.77
2:C:167:THR:HG22	3:E:184:VAL:HG12	1.66	0.77
3:H:116:ASP:O	5:H:302:HOH:O	2.02	0.76
1:B:478:LYS:HZ2	1:B:486:PHE:CB	1.98	0.76
3:H:84:ASN:OD1	5:H:303:HOH:O	2.03	0.75
2:C:85:GLU:OE2	5:C:304:HOH:O	2.03	0.75
1:A:467:ASP:OD2	5:A:703:HOH:O	2.04	0.74
1:B:478:LYS:NZ	1:B:486:PHE:CB	2.51	0.73
2:C:124:PRO:N	2:C:124:PRO:C	2.47	0.73
1:B:478:LYS:HZ2	1:B:486:PHE:HB3	1.51	0.72
3:H:167:VAL:HG11	3:H:195:SER:HB2	1.71	0.72
2:C:203:GLU:OE2	5:C:305:HOH:O	2.08	0.72
2:D:169:PRO:N	2:D:169:PRO:C	2.47	0.72
2:C:83:GLU:OE1	5:C:302:HOH:O	2.08	0.71
2:D:125:PRO:HD3	2:D:137:LEU:HD21	1.71	0.71
2:C:120:VAL:O	2:C:209:LYS:HD2	1.90	0.71
3:E:138:PRO:HG3	3:E:224:LYS:HG2	1.71	0.71
1:A:449:TYR:O	5:A:704:HOH:O	2.09	0.71
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.73	0.70
1:B:478:LYS:HZ3	1:B:486:PHE:HB3	1.56	0.70
1:B:343:ASN:HD21	4:B:601:NAG:C2	2.04	0.69
2:C:127:SER:O	2:C:127:SER:OG	2.10	0.69
2:D:140:LEU:HD21	3:H:194:SER:HB2	1.73	0.69
1:A:480:CYS:O	5:A:705:HOH:O	2.11	0.69
1:B:451:TYR:O	5:B:703:HOH:O	2.10	0.68
3:E:225:LYS:HD2	3:E:225:LYS:N	2.08	0.68
3:H:137:PHE:HB3	3:H:138:PRO:HD2	1.74	0.68
1:B:405:ASP:OD1	5:B:705:HOH:O	2.11	0.68
3:H:140:ALA:HB3	3:H:141:PRO:HD3	1.76	0.67
2:C:33:TYR:CZ	3:E:110:LEU:HD22	2.30	0.67
3:H:189:GLY:O	5:H:305:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:LEU:HD23	2:C:86:ALA:HB2	1.76	0.67
3:E:138:PRO:CG	3:E:224:LYS:HE2	2.25	0.67
2:D:125:PRO:HD3	2:D:137:LEU:CD2	2.25	0.66
1:A:364:ASP:O	1:A:367:VAL:HG22	1.95	0.66
3:E:225:LYS:H	3:E:225:LYS:CD	2.08	0.66
2:C:65:SER:O	2:C:75:LEU:HD12	1.95	0.66
1:B:393:THR:OG1	5:B:706:HOH:O	2.12	0.65
2:D:126:SER:O	2:D:130:LEU:HD12	1.96	0.65
2:D:44:THR:HG22	2:D:45:ALA:O	1.97	0.64
3:H:12:VAL:HG11	3:H:86:LEU:HD13	1.81	0.63
2:C:154:LYS:HZ2	2:C:158:SER:HB3	1.63	0.63
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.82	0.62
3:H:12:VAL:HG22	3:H:16:ARG:HB2	1.84	0.60
2:C:138:VAL:HG22	2:C:182:TYR:CD1	2.35	0.60
3:E:180:THR:HG22	3:E:195:SER:OG	2.02	0.60
3:E:138:PRO:HG2	3:E:224:LYS:HE2	1.84	0.60
2:D:158:SER:OG	2:D:159:PRO:HD2	2.02	0.59
3:H:77:ASN:ND2	5:H:307:HOH:O	2.31	0.59
1:B:478:LYS:HD2	1:B:487:ASN:HB2	1.85	0.59
1:A:403:ARG:NE	5:A:706:HOH:O	2.36	0.59
1:B:373:PRO:O	5:B:707:HOH:O	2.17	0.59
2:C:167:THR:HG23	3:E:184:VAL:HG12	1.85	0.58
1:A:343:ASN:HD22	4:A:601:NAG:C1	2.06	0.57
1:B:478:LYS:HD2	1:B:486:PHE:O	2.05	0.57
2:C:154:LYS:NZ	2:C:158:SER:HB3	2.18	0.57
2:C:141:ILE:HG22	2:C:144:PHE:CE1	2.39	0.57
3:E:199:VAL:HG11	3:E:209:TYR:OH	2.05	0.56
1:B:405:ASP:CG	5:B:705:HOH:O	2.48	0.56
2:C:210:THR:O	2:C:210:THR:HG22	2.05	0.56
2:D:87:ASP:OD1	2:D:107:ARG:NE	2.39	0.56
3:H:165:VAL:HG12	3:H:193:LEU:HD21	1.88	0.55
2:D:146:PRO:HD2	2:D:203:GLU:HG3	1.87	0.55
2:D:33:TYR:O	2:D:68:LYS:NZ	2.39	0.55
2:D:1:GLN:NE2	2:D:1:GLN:H3	2.04	0.55
2:D:49:LEU:HD21	2:D:64:PHE:CD2	2.42	0.54
2:C:63:ARG:NH2	2:C:84:ASP:OD1	2.40	0.54
1:A:357:ARG:NH1	1:A:396:TYR:OH	2.41	0.53
2:C:158:SER:OG	5:C:306:HOH:O	2.19	0.52
2:C:137:LEU:HD13	2:C:183:LEU:HD23	1.90	0.52
3:E:175:THR:O	3:E:175:THR:OG1	2.27	0.52
3:E:12:VAL:HG11	3:E:86:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:91:THR:HG23	3:H:125:THR:HA	1.91	0.52
2:C:108:LEU:C	2:C:108:LEU:HD23	2.36	0.51
2:C:171:LYS:H	2:C:171:LYS:HE2	1.76	0.51
3:E:93:LEU:HD23	3:E:95:TYR:CZ	2.45	0.51
3:E:203:SER:HB3	3:E:228:PRO:HG3	1.92	0.51
2:C:208:GLU:O	2:C:209:LYS:HG2	2.11	0.51
3:E:138:PRO:HG3	3:E:224:LYS:HG3	1.90	0.51
3:H:94:TYR:O	3:H:121:GLY:HA2	2.11	0.50
3:E:203:SER:HB3	3:E:228:PRO:CG	2.41	0.50
1:B:376:THR:OG1	5:B:702:HOH:O	2.10	0.50
1:B:393:THR:HG1	1:B:518:LEU:H	1.59	0.50
2:D:63:ARG:HB2	2:D:78:THR:HG22	1.92	0.50
2:C:138:VAL:HG22	2:C:182:TYR:CE1	2.46	0.50
3:E:216:LYS:N	3:E:216:LYS:HD3	2.26	0.50
1:B:474:GLN:HG2	1:B:480:CYS:SG	2.52	0.50
3:H:136:VAL:HA	3:H:156:LEU:O	2.12	0.50
2:D:1:GLN:NE2	2:D:1:GLN:N	2.59	0.49
3:E:12:VAL:HG22	3:E:13:GLN:N	2.26	0.49
3:E:225:LYS:N	3:E:225:LYS:CD	2.73	0.49
2:D:138:VAL:HG13	2:D:182:TYR:CE1	2.47	0.49
1:B:403:ARG:NE	5:B:710:HOH:O	2.42	0.49
3:E:43:LYS:HA	3:E:43:LYS:HE2	1.94	0.49
3:H:197:VAL:HG12	3:H:199:VAL:HG13	1.93	0.49
2:C:35:VAL:N	2:C:53:ASN:OD1	2.28	0.49
2:D:168:THR:HG21	3:H:42:GLY:HA3	1.95	0.49
2:C:138:VAL:HG13	2:C:182:TYR:CE1	2.47	0.49
3:E:151:ALA:HB2	3:E:199:VAL:HG12	1.94	0.49
3:E:99:ASP:OD1	3:E:100:ASN:N	2.46	0.48
3:E:20:LEU:HD22	3:E:122:THR:HG21	1.96	0.48
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.96	0.48
1:B:400:PHE:HZ	1:B:410:ILE:HG12	1.78	0.47
2:C:1:GLN:N	2:C:1:GLN:CD	2.71	0.47
1:B:343:ASN:CG	4:B:601:NAG:C1	2.78	0.47
2:C:56:ARG:HB3	2:C:60:VAL:HG23	1.96	0.47
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.50	0.46
2:D:124:PRO:HA	2:D:137:LEU:CD2	2.46	0.46
1:A:367:VAL:HG23	4:A:601:NAG:H81	1.98	0.46
3:E:210:ILE:HA	3:E:224:LYS:O	2.15	0.46
2:D:1:GLN:H3	2:D:1:GLN:CD	2.24	0.46
3:H:99:ASP:OD1	3:H:100:ASN:N	2.47	0.46
1:B:449:TYR:CD2	3:E:65:LYS:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:LEU:HD13	3:E:191:TYR:CZ	2.51	0.46
2:D:192:SER:OG	2:D:193:HIS:N	2.48	0.45
3:E:34:MET:HB3	3:E:79:LEU:HD22	1.98	0.45
2:C:56:ARG:HB3	2:C:60:VAL:CG2	2.46	0.45
2:C:63:ARG:HB2	2:C:78:THR:HG22	1.98	0.45
1:B:403:ARG:NH2	5:B:710:HOH:O	2.48	0.45
3:E:193:LEU:HD12	3:E:193:LEU:C	2.42	0.45
1:B:342:PHE:HB2	4:B:601:NAG:H82	1.98	0.44
1:A:367:VAL:O	4:A:601:NAG:H83	2.17	0.44
2:C:158:SER:N	5:C:306:HOH:O	2.50	0.44
1:A:448:ASN:OD1	1:A:498:ARG:NH1	2.35	0.44
2:C:145:TYR:OH	5:C:307:HOH:O	2.21	0.44
2:D:49:LEU:O	2:D:57:PRO:HD2	2.18	0.44
1:A:354:ASN:O	1:A:398:ASP:HA	2.18	0.44
3:E:138:PRO:HG3	3:E:224:LYS:HE2	2.00	0.44
2:C:164:VAL:HG22	2:C:183:LEU:CD1	2.48	0.44
3:H:137:PHE:O	3:H:156:LEU:N	2.51	0.44
2:D:153:TRP:CD1	2:D:164:VAL:HG11	2.53	0.43
3:E:199:VAL:CG1	3:E:209:TYR:OH	2.66	0.43
2:C:190:TRP:O	2:C:213:PRO:HG3	2.18	0.43
3:E:6:GLU:OE1	3:E:121:GLY:N	2.50	0.43
1:A:421:TYR:C	1:A:461:LEU:HD12	2.43	0.43
1:B:487:ASN:HA	1:B:489:TYR:CE1	2.53	0.43
1:A:355:ARG:HD3	1:A:396:TYR:CD2	2.54	0.43
3:H:12:VAL:CG2	3:H:16:ARG:HB2	2.49	0.43
2:C:160:VAL:CG1	2:C:160:VAL:O	2.67	0.43
2:D:123:PHE:HZ	3:H:141:PRO:C	2.27	0.43
2:D:79:GLY:O	2:D:80:LEU:C	2.62	0.43
2:C:200:VAL:O	2:C:206:THR:HA	2.19	0.43
3:E:83:MET:HB3	3:E:86:LEU:HD21	2.01	0.43
3:E:215:HIS:CD2	3:E:217:PRO:HD2	2.54	0.43
2:D:1:GLN:N	2:D:1:GLN:CD	2.77	0.42
2:D:129:GLU:CD	2:D:136:THR:HG22	2.44	0.42
3:E:154:GLY:HA3	3:E:195:SER:O	2.19	0.42
1:A:370:ASN:HD21	1:A:436:TRP:CG	2.37	0.42
2:C:87:ASP:OD1	2:C:107:ARG:NE	2.47	0.42
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.01	0.42
2:C:29:ILE:HG22	2:C:70:GLY:O	2.19	0.42
1:B:389:ASP:OD2	1:B:528:LYS:HD2	2.20	0.42
2:C:139:CYS:HB2	2:C:153:TRP:CH2	2.54	0.42
2:C:183:LEU:HD21	2:C:185:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:VAL:HG21	3:E:115:MET:HE3	2.01	0.42
3:E:134:PRO:HB3	3:E:160:TYR:HB3	2.00	0.42
1:A:349:SER:OG	1:A:451:TYR:HA	2.20	0.42
1:B:410:ILE:N	1:B:410:ILE:HD12	2.35	0.42
2:C:149:VAL:HG22	2:C:200:VAL:HG13	2.00	0.42
2:C:172:GLN:CA	2:C:172:GLN:HE21	2.32	0.42
2:C:191:LYS:HD2	2:C:191:LYS:C	2.45	0.42
3:E:157:VAL:HG11	3:E:165:VAL:HG11	2.02	0.42
2:D:17:ARG:NH1	5:D:305:HOH:O	2.40	0.42
2:C:60:VAL:HG23	2:C:60:VAL:O	2.20	0.42
2:C:164:VAL:HG22	2:C:183:LEU:HD13	2.01	0.42
1:A:342:PHE:CZ	1:A:368:LEU:HD22	2.55	0.41
2:C:41:LEU:HB3	2:C:42:PRO:HD2	2.02	0.41
3:E:27:PHE:CE2	3:E:98:LYS:HD2	2.55	0.41
2:C:154:LYS:HZ2	2:C:158:SER:CB	2.30	0.41
1:B:342:PHE:CZ	1:B:511:VAL:HG11	2.55	0.41
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.55	0.41
2:D:84:ASP:O	2:D:108:LEU:HD22	2.21	0.41
3:E:140:ALA:HB1	3:E:141:PRO:HD2	2.02	0.41
2:D:129:GLU:OE2	2:D:136:THR:HG22	2.19	0.41
2:D:202:HIS:O	2:D:203:GLU:C	2.64	0.41
3:H:83:MET:HE1	3:H:124:VAL:HG21	2.03	0.41
1:A:370:ASN:OD1	1:A:370:ASN:C	2.63	0.41
1:B:502:GLY:O	1:B:506:GLN:HG3	2.21	0.41
2:C:161:LYS:HA	2:C:161:LYS:HD2	1.67	0.41
1:B:342:PHE:CE2	1:B:511:VAL:HG11	2.56	0.41
2:D:140:LEU:HB3	3:H:181:PHE:CZ	2.56	0.40
3:H:68:PHE:C	3:H:69:ILE:HG13	2.45	0.40
3:H:140:ALA:HB3	3:H:141:PRO:CD	2.49	0.40
2:D:189:GLN:O	2:D:196:TYR:OH	2.35	0.40
1:B:402:ILE:CD1	1:B:410:ILE:HD13	2.52	0.40
3:H:12:VAL:O	3:H:126:VAL:HA	2.21	0.40
3:H:193:LEU:C	3:H:193:LEU:HD12	2.46	0.40
2:D:166:THR:HG22	2:D:181:SER:OG	2.21	0.40
2:D:174:ASN:HD22	2:D:174:ASN:HA	1.73	0.40
1:B:399:SER:O	1:B:400:PHE:HB3	2.21	0.40
3:E:140:ALA:HB1	3:E:229:LYS:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:762:HOH:O	5:B:764:HOH:O[1_455]	1.88	0.32
5:D:310:HOH:O	5:D:339:HOH:O[4_455]	2.06	0.14
5:B:740:HOH:O	5:B:764:HOH:O[1_455]	2.07	0.13
5:D:321:HOH:O	5:D:338:HOH:O[4_555]	2.19	0.01

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	193/195 (99%)	185 (96%)	8 (4%)	0	100	100
1	B	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
2	C	206/214 (96%)	189 (92%)	17 (8%)	0	100	100
2	D	201/214 (94%)	188 (94%)	13 (6%)	0	100	100
3	E	209/229 (91%)	190 (91%)	19 (9%)	0	100	100
3	H	172/229 (75%)	164 (95%)	8 (5%)	0	100	100
All	All	1174/1276 (92%)	1103 (94%)	71 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	170/170 (100%)	170 (100%)	0	100	100
1	B	170/170 (100%)	169 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	175/179 (98%)	163 (93%)	12 (7%)	14	32
2	D	170/179 (95%)	162 (95%)	8 (5%)	23	48
3	E	182/192 (95%)	170 (93%)	12 (7%)	15	34
3	H	150/192 (78%)	147 (98%)	3 (2%)	48	74
All	All	1017/1082 (94%)	981 (96%)	36 (4%)	32	59

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	1	GLN
2	D	3	VAL
2	D	112	ARG
2	D	133	ASN
2	D	134	LYS
2	D	154	LYS
2	D	161	LYS
2	D	174	ASN
3	H	3	GLN
3	H	166	THR
3	H	167	VAL
1	B	493	ARG
2	C	1	GLN
2	C	115	LYS
2	C	119	SER
2	C	133	ASN
2	C	154	LYS
2	C	158	SER
2	C	160	VAL
2	C	171	LYS
2	C	172	GLN
2	C	174	ASN
2	C	188	GLU
2	C	194	LYS
3	E	165	VAL
3	E	175	THR
3	E	199	VAL
3	E	206	THR
3	E	207	GLN
3	E	208	THR
3	E	211	CYS
3	E	212	ASN

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Mol	Chain	Res	Type
3	E	222	VAL
3	E	225	LYS
3	E	227	GLU
3	E	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
2	D	1	GLN
2	D	174	ASN
2	D	202	HIS
3	H	179	HIS
1	B	343	ASN
1	B	409	GLN
1	B	505	HIS
2	C	16	GLN
2	C	39	GLN
2	C	172	GLN
3	E	120	GLN
3	E	207	GLN
3	E	212	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 ⓘ

There are no oligosaccharides in this entry.

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$
4	NAG	B	601	-	14,14,15	1.05	0	17,19,21	2.27	6 (35%)
4	NAG	A	601	1	14,14,15	1.21	2 (14%)	17,19,21	3.24	11 (64%)

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	B	601	-	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O5-C1	-3.18	1.38	1.43
4	A	601	NAG	C2-N2	-2.02	1.42	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	O5-C1-C2	-8.80	97.68	111.29
4	B	601	NAG	C1-O5-C5	5.99	120.21	112.19
4	A	601	NAG	C1-O5-C5	5.03	118.93	112.19
4	A	601	NAG	O3-C3-C2	3.65	116.99	109.40
4	A	601	NAG	C3-C4-C5	-3.36	104.13	110.23
4	A	601	NAG	O7-C7-N2	3.14	127.53	121.98
4	B	601	NAG	O3-C3-C2	-3.05	103.06	109.40
4	B	601	NAG	O4-C4-C5	2.94	116.57	109.32
4	B	601	NAG	O3-C3-C4	-2.76	103.87	110.38
4	B	601	NAG	O6-C6-C5	2.70	120.54	111.33
4	A	601	NAG	C1-C2-N2	2.69	114.67	110.43
4	A	601	NAG	C2-N2-C7	2.58	126.35	122.90
4	A	601	NAG	C6-C5-C4	-2.52	106.84	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	O4-C4-C5	2.41	115.27	109.32
4	A	601	NAG	O3-C3-C4	-2.36	104.82	110.38
4	A	601	NAG	C8-C7-N2	-2.35	112.23	116.12
4	B	601	NAG	C4-C3-C2	2.33	114.44	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	5	0
4	A	601	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/195 (100%)	0.05	2 (1%) 79 76	13, 23, 36, 52	0
1	B	195/195 (100%)	0.29	9 (4%) 37 32	15, 25, 47, 71	0
2	C	210/214 (98%)	0.76	21 (10%) 12 9	19, 34, 50, 59	0
2	D	203/214 (94%)	0.84	34 (16%) 4 3	16, 29, 62, 99	0
3	E	215/229 (93%)	0.58	20 (9%) 14 11	14, 26, 46, 65	0
3	H	178/229 (77%)	0.37	14 (7%) 18 14	13, 22, 56, 70	0
All	All	1196/1276 (93%)	0.49	100 (8%) 17 13	13, 26, 54, 99	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	160	VAL	6.9
3	E	208	THR	6.3
2	D	133	ASN	5.8
2	D	132	ALA	5.7
3	H	139	LEU	5.6
3	E	199	VAL	5.3
2	C	156	ASP	5.3
3	E	205	GLY	4.9
1	B	456	PHE	4.8
3	E	204	LEU	4.8
3	H	138	PRO	4.7
1	B	478	LYS	4.7
1	B	473	TYR	4.5
3	H	140	ALA	4.5
1	B	475	ALA	4.4
3	E	212	ASN	4.3
3	E	211	CYS	4.3
2	D	116	ALA	4.2
3	E	177	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	H	141	PRO	4.1
3	E	207	GLN	4.1
2	C	155	ALA	4.0
3	E	206	THR	4.0
2	C	188	GLU	3.9
2	D	174	ASN	3.9
2	C	157	SER	3.7
3	H	135	SER	3.6
1	B	477	ASN	3.6
3	E	151	ALA	3.5
2	C	127	SER	3.4
2	C	161	LYS	3.4
3	E	175	THR	3.3
2	C	143	ASP	3.3
2	D	150	THR	3.3
2	C	206	THR	3.3
2	D	193	HIS	3.3
2	C	192	SER	3.3
2	D	188	GLU	3.2
2	C	132	ALA	3.2
2	D	149	VAL	3.1
2	D	175	ASN	3.1
2	D	162	ALA	3.1
2	D	194	LYS	3.1
2	D	192	SER	3.1
2	D	190	TRP	3.0
3	H	168	SER	3.0
2	D	185	LEU	2.9
2	D	121	THR	2.9
2	D	163	GLY	2.9
1	B	373	PRO	2.8
2	D	160	VAL	2.8
3	E	176	SER	2.7
2	D	140	LEU	2.6
3	E	227	GLU	2.6
1	B	474	GLN	2.6
2	C	62	ASP	2.6
1	A	388	ASN	2.6
2	C	172	GLN	2.6
3	H	202	SER	2.6
2	D	153	TRP	2.5
2	D	195	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	210	THR	2.5
2	D	180	SER	2.5
3	H	167	VAL	2.5
3	H	161	PHE	2.5
2	D	126	SER	2.4
2	D	173	SER	2.4
2	D	164	VAL	2.4
2	D	156	ASP	2.4
2	C	190	TRP	2.4
2	D	201	THR	2.4
3	E	203	SER	2.4
2	C	207	VAL	2.4
3	H	196	VAL	2.4
1	A	396	TYR	2.3
2	D	158	SER	2.3
2	D	131	GLN	2.3
3	E	198	THR	2.2
1	B	493	ARG	2.2
2	D	129	GLU	2.2
2	D	191	LYS	2.2
3	H	194	SER	2.2
3	E	168	SER	2.2
2	C	193	HIS	2.1
2	D	181	SER	2.1
3	H	201	SER	2.1
2	C	194	LYS	2.1
2	C	1	GLN	2.1
2	D	197	SER	2.1
3	E	152	ALA	2.1
1	B	479	PRO	2.1
2	D	159	PRO	2.1
2	D	1	GLN	2.1
2	C	182	TYR	2.1
3	E	185	LEU	2.0
3	H	184	VAL	2.0
3	E	225	LYS	2.0
2	C	214	THR	2.0
3	H	164	PRO	2.0
3	E	210	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	601	14/15	0.57	0.23	20,20,20,20	0
4	NAG	B	601	14/15	0.85	0.11	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.