



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:37 AM UTC

PDB ID : 3NWF / pdb_00003nwf
Title : Glycoprotein B from Herpes simplex virus type 1, low-pH
Authors : Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on : 2010-07-09
Resolution : 3.00 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

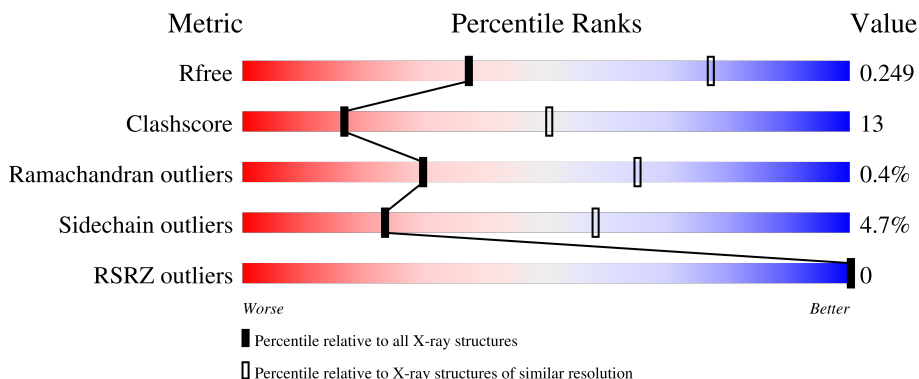
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	703	
1	B	703	
1	C	703	
1	D	703	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19321 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.

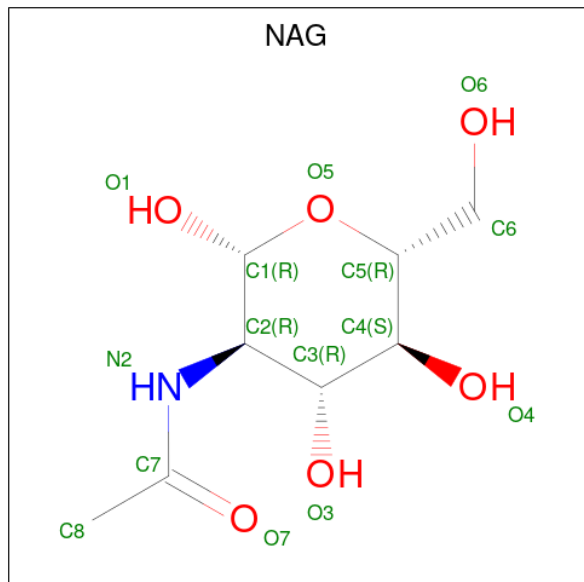
- Molecule 1 is a protein called Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4814	3040	845	907	22			
1	B	596	Total	C	N	O	S	0	1	0
			4762	3012	837	891	22			
1	C	603	Total	C	N	O	S	0	0	0
			4727	2985	814	907	21			
1	D	605	Total	C	N	O	S	0	0	0
			4813	3036	841	914	22			

There are 20 discrepancies between the modelled and reference sequences:

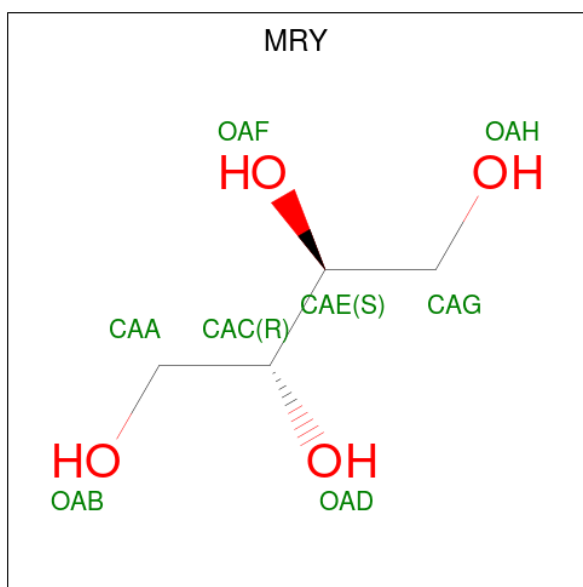
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	expression tag	UNP P06437
C	29	PRO	-	expression tag	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	expression tag	UNP P06437
D	29	PRO	-	expression tag	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

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



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

- Molecule 3 is MESO-ERYTHRITOL (CCD ID: MRY) (formula: $C_4H_{10}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

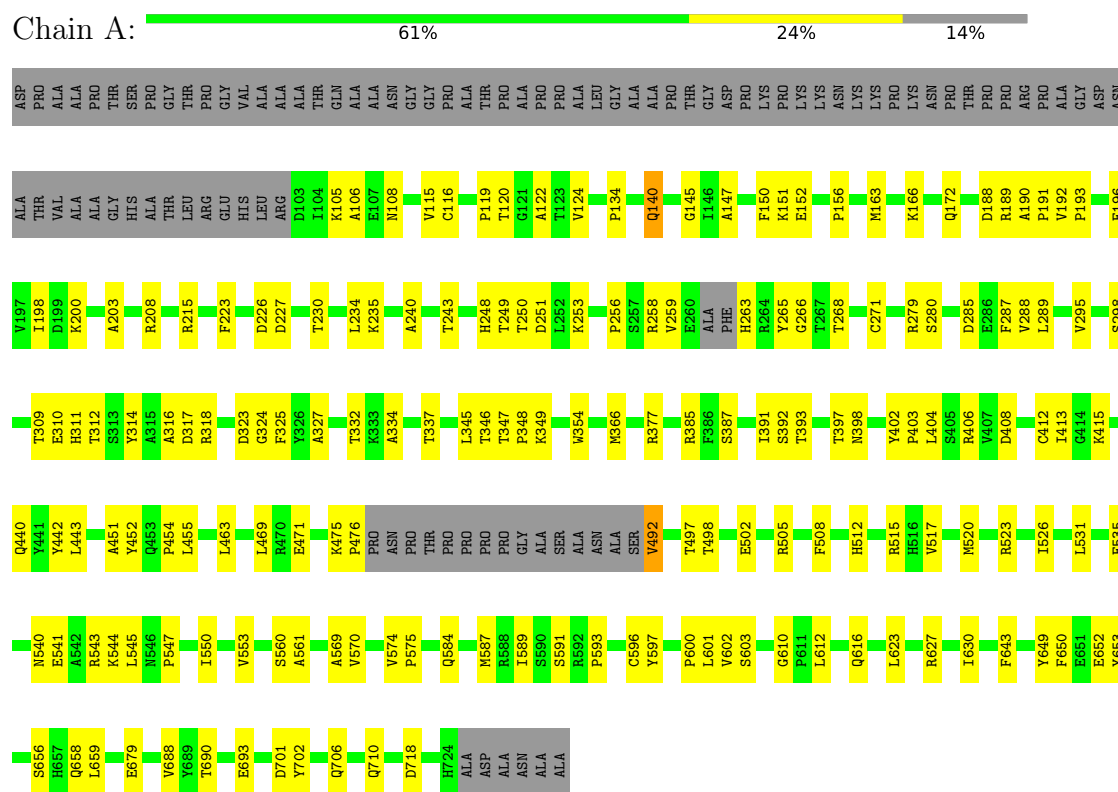
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	17	Total	O	0	0
			17	17		
5	C	12	Total	O	0	0
			12	12		
5	D	15	Total	O	0	0
			15	15		

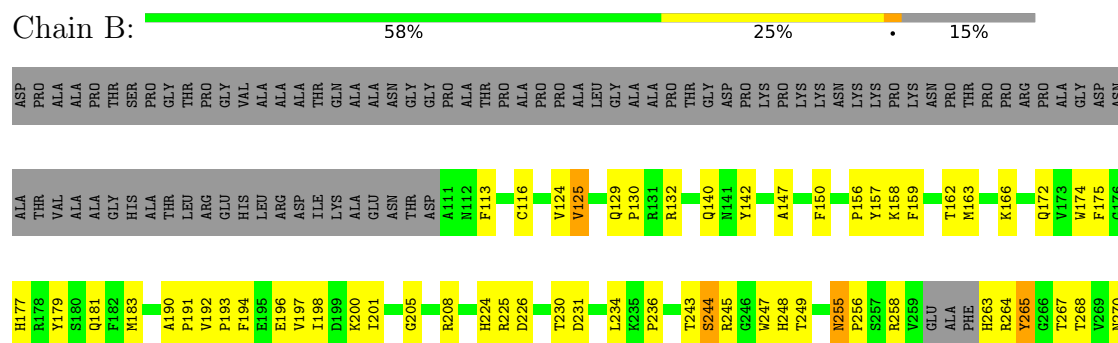
3 Residue-property plots

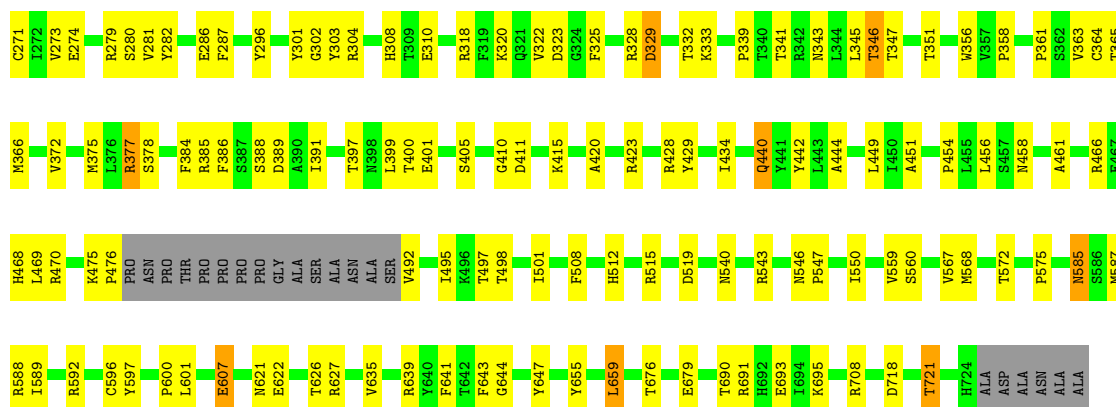
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Envelope glycoprotein B



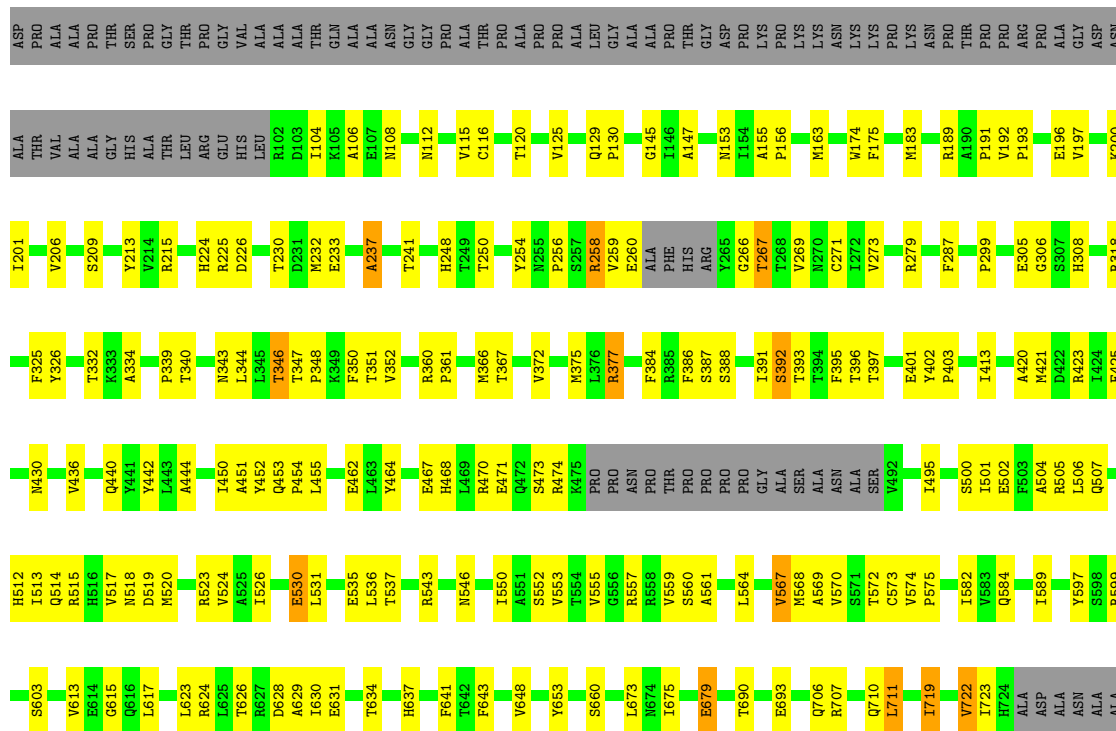
• Molecule 1: Envelope glycoprotein B





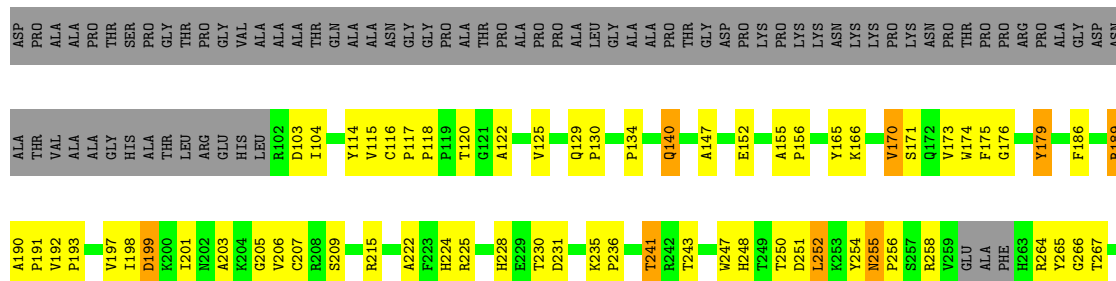
• Molecule 1: Envelope glycoprotein B

Chain C: 58% 26% 14%



• Molecule 1: Envelope glycoprotein B

Chain D: 57% 26% 14%



T572	C573	V574	I582	M587	L601	V602	S603	Q609	V613	Q616	R627	T634	V635	R638	R639	Y640	F641	V648	Y649	Y653	Q658	L659	T690	E693	V705	Q706	N709	Q710	T721	V722	I723	HIS	ALA	ASP	ALA	ASN	ALA	ALA											
■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■								
C271	S280	V281	Y282	P283	F287	S298	P299	F300	Y301	S307	H308	T309	E310	H311	T312	S313	F319	K320	Q321	V322	D323	G324	F325	Y326	A327	R328	T332	K333	A334	R335	A336	P339	T340	T341	R342	N343	L344	L345	T346	K349	F350	T351	T365	M366	T367	K368	M375	L376	R377
S378	G382	S383	F384	R385	F386	D389	F395	T396	T397	N398	L399	T400	E401	Y402	P403	R406	V407	L409	C412	I413	A420	R423	A426	N430	A431	T432	H433	Q438	P439	Q440	Y441	Y442	L443	A444	F448	L449	T450	A451	Q453	R470	E471	Q472	S473	R474	K475				
P476	P477	ASN	PRO	THR	PRO	PRO	PRO	PRO	GLY	ALA	SER	ALA	ASN	ALA	SER	V492	E493	R494	I495	S500	I501	D502	F503	A504	R505	L506	Q507	N511	H512	R515	D519	G522	I526	A527	W528	L531	Q532	E535	L536	T537	N546	I550	R558	V559	S560	M568			

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	117.80Å 117.80Å 318.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.54 – 3.00 41.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.54-3.00) 93.3 (41.54-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.197 , 0.249 0.194 , 0.249	Depositor DCC
R_{free} test set	5715 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.460 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19321	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5300e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, MRY, 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	0.29	0/4931	0.72	2/6708 (0.0%)
1	B	0.29	0/4884	0.72	1/6644 (0.0%)
1	C	0.28	0/4840	0.71	1/6599 (0.0%)
1	D	0.29	0/4930	0.72	2/6713 (0.0%)
All	All	0.29	0/19585	0.72	6/26664 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ASN	CA-C-N	5.50	126.71	119.84
1	D	255	ASN	C-N-CA	5.50	126.71	119.84
1	B	198	ILE	N-CA-C	5.38	115.47	110.42
1	C	305	GLU	CB-CA-C	-5.19	109.62	115.79
1	A	610	GLY	CA-C-N	5.03	125.04	120.21
1	A	610	GLY	C-N-CA	5.03	125.04	120.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4814	0	4593	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4762	0	4552	123	0
1	C	4727	0	4425	127	0
1	D	4813	0	4565	134	0
2	A	42	0	39	2	0
2	B	14	0	13	0	0
2	C	42	0	39	0	0
2	D	14	0	13	0	0
3	A	8	0	10	0	0
3	B	8	0	10	3	0
4	A	1	0	0	0	0
5	A	32	0	0	2	0
5	B	17	0	0	2	0
5	C	12	0	0	0	0
5	D	15	0	0	0	0
All	All	19321	0	18259	479	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 13.

All (479) 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:116:CYS:HB3	1:C:560:SER:HB2	1.52	0.90
1:D:140:GLN:HE21	1:D:378:SER:HB2	1.37	0.90
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.52	0.89
1:A:189:ARG:HB2	1:A:349:LYS:HE2	1.54	0.88
1:A:397:THR:HG21	1:A:442:TYR:HB3	1.58	0.83
1:C:377:ARG:HD3	1:C:384:PHE:CD1	2.12	0.83
1:A:412:CYS:HA	1:A:415:LYS:HE2	1.64	0.80
1:B:265:TYR:C	1:B:265:TYR:HD2	1.92	0.78
1:C:543:ARG:HB3	1:C:550:ILE:HG21	1.67	0.77
1:D:176:GLY:HA3	1:D:179:TYR:HE1	1.50	0.75
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.69	0.75
1:A:193:PRO:HD2	1:A:196:GLU:HB3	1.70	0.74
1:A:325:PHE:HE2	1:A:327:ALA:HB2	1.54	0.73
1:B:364:CYS:SG	1:B:410:GLY:HA2	2.29	0.72
1:C:115:VAL:HG22	1:C:623:LEU:HB2	1.72	0.72
1:A:597:TYR:HA	1:A:630:ILE:HA	1.72	0.71
1:D:587:MET:HE2	1:D:653:TYR:HA	1.73	0.70
1:B:265:TYR:C	1:B:265:TYR:CD2	2.67	0.70
1:C:174:TRP:HB2	1:C:183:MET:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ALA:HB2	1:C:452:TYR:HD1	1.58	0.69
1:D:166:LYS:HE3	1:D:192:VAL:HG22	1.74	0.69
1:A:140:GLN:HA	2:A:1141:NAG:H82	1.75	0.68
1:B:243:THR:OG1	3:B:4000:MRY:HAA2	1.92	0.68
1:C:397:THR:HG21	1:C:442:TYR:HB3	1.74	0.68
1:C:213:TYR:HE1	1:C:215:ARG:HB2	1.57	0.68
1:C:366:MET:HE2	1:C:495:ILE:HD12	1.76	0.68
1:D:140:GLN:NE2	1:D:378:SER:HB2	2.07	0.66
1:A:166:LYS:HB2	1:A:190:ALA:HB3	1.77	0.66
1:C:679:GLU:CD	1:C:679:GLU:H	2.02	0.66
1:B:194:PHE:CG	1:B:320:LYS:HD2	2.31	0.65
1:D:116:CYS:HB3	1:D:560:SER:HB3	1.77	0.65
1:D:176:GLY:HA3	1:D:179:TYR:CE1	2.29	0.65
1:D:401:GLU:HB2	1:D:474:ARG:O	1.96	0.65
1:C:174:TRP:CB	1:C:183:MET:HE2	2.27	0.65
1:A:543:ARG:HB3	1:A:550:ILE:HG21	1.78	0.65
1:A:600:PRO:O	1:A:616:GLN:HB2	1.96	0.65
1:B:466:ARG:NH2	1:B:470:ARG:HB2	2.12	0.64
1:D:170:VAL:HG13	1:D:186:PHE:HB3	1.79	0.64
1:B:559:VAL:HG12	1:B:572:THR:HA	1.79	0.64
1:D:705:VAL:HG12	1:D:709:ASN:ND2	2.12	0.64
1:B:567:VAL:HG22	1:B:568:MET:H	1.63	0.64
1:D:377:ARG:HD3	1:D:384:PHE:CE1	2.33	0.64
1:D:690:THR:HB	1:D:693:GLU:HG3	1.79	0.64
1:C:531:LEU:O	1:C:535:GLU:HG2	1.99	0.63
1:D:377:ARG:HD3	1:D:384:PHE:CD1	2.34	0.63
1:B:601:LEU:HD22	1:B:627:ARG:HD3	1.82	0.62
1:C:572:THR:HG22	1:C:573:CYS:H	1.64	0.62
1:C:326:TYR:CE2	1:C:339:PRO:HB3	2.34	0.62
1:C:387:SER:HA	1:C:393:THR:O	1.99	0.61
1:C:230:THR:O	1:C:232:MET:HG3	2.01	0.61
1:C:192:VAL:HG11	1:C:201:ILE:HD11	1.83	0.61
1:C:372:VAL:HG11	1:C:375:MET:HE2	1.82	0.61
1:D:225:ARG:HA	1:D:254:TYR:CD2	2.35	0.61
1:B:230:THR:HG22	1:B:231:ASP:N	2.16	0.61
1:D:403:PRO:HG3	1:D:476:PRO:HB3	1.81	0.60
1:D:476:PRO:HB2	1:D:477:PRO:HD3	1.84	0.60
1:A:318:ARG:HD2	1:A:346:THR:O	2.01	0.60
1:B:172:GLN:OE1	1:B:183:MET:HE2	2.02	0.60
1:A:408:ASP:HB2	1:A:492:VAL:HG13	1.84	0.60
1:A:443:LEU:O	2:A:1398:NAG:H81	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASP:HB3	1:D:582:ILE:HD13	1.83	0.60
1:A:603:SER:HB3	1:A:612:LEU:HD21	1.85	0.59
1:C:213:TYR:CE1	1:C:215:ARG:HB2	2.37	0.59
1:D:225:ARG:HG2	1:D:254:TYR:CD1	2.36	0.59
1:C:520:MET:O	1:C:524:VAL:HG23	2.01	0.59
1:A:253:LYS:HD3	1:A:268:THR:HG21	1.84	0.59
1:B:304:ARG:HH11	1:B:341:THR:HG23	1.68	0.59
1:C:287:PHE:HB3	1:C:299:PRO:HG3	1.85	0.59
1:D:401:GLU:HG2	1:D:441:TYR:O	2.02	0.59
1:B:201:ILE:O	1:B:205:GLY:HA2	2.03	0.59
1:C:259:VAL:HG23	1:C:260:GLU:OE1	2.03	0.59
1:B:372:VAL:HG11	1:B:375:MET:HE2	1.84	0.59
1:D:197:VAL:HA	1:D:201:ILE:HD12	1.84	0.59
1:D:256:PRO:HG2	1:D:264:ARG:O	2.03	0.59
1:B:540:ASN:O	1:B:543:ARG:HG2	2.02	0.58
1:B:191:PRO:HG3	1:B:347:THR:O	2.03	0.58
1:B:256:PRO:HG3	1:B:264:ARG:O	2.03	0.58
1:C:237:ALA:HA	1:C:248:HIS:CE1	2.39	0.58
1:D:206:VAL:HG11	1:D:231:ASP:HB3	1.85	0.58
1:A:601:LEU:HD23	1:A:627:ARG:HD3	1.86	0.57
1:A:124:VAL:HG22	1:A:569:ALA:HA	1.86	0.57
1:B:142:TYR:CD2	1:B:378:SER:HB3	2.38	0.57
1:C:237:ALA:HA	1:C:248:HIS:ND1	2.19	0.57
1:C:470:ARG:O	1:C:473:SER:HB3	2.03	0.57
1:A:223:PHE:HB2	1:A:226:ASP:HA	1.87	0.57
1:B:248:HIS:HA	1:B:271:CYS:O	2.04	0.57
1:A:256:PRO:HD3	1:A:266:GLY:HA3	1.86	0.57
1:D:493:GLU:HG2	1:D:494:ARG:H	1.69	0.57
1:B:420:ALA:HA	1:B:423:ARG:NH2	2.18	0.57
1:B:458:ASN:HA	1:B:461:ALA:HB2	1.87	0.57
1:A:172:GLN:OE1	1:A:265:TYR:HB3	2.05	0.56
1:C:392:SER:O	1:C:505:ARG:HA	2.05	0.56
1:C:393:THR:HG23	1:C:504:ALA:HB1	1.87	0.56
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.87	0.56
1:B:245:ARG:HA	3:B:4000:MRY:HAG2	1.87	0.56
1:C:196:GLU:O	1:C:200:LYS:HB2	2.05	0.56
1:C:500:SER:OG	1:C:502:GLU:HG2	2.06	0.56
1:B:515:ARG:O	1:B:519:ASP:HB2	2.05	0.56
1:C:226:ASP:OD2	1:C:267:THR:HB	2.05	0.56
1:D:638:ARG:HB3	1:D:649:TYR:OH	2.04	0.56
1:C:567:VAL:HG13	1:C:568:MET:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PHE:CE2	1:A:327:ALA:HB2	2.38	0.55
1:A:393:THR:HG22	1:A:505:ARG:HG2	1.87	0.55
1:B:384:PHE:CE2	1:B:399:LEU:HA	2.41	0.55
1:D:384:PHE:CE2	1:D:399:LEU:HA	2.41	0.55
1:D:420:ALA:HA	1:D:423:ARG:NH2	2.21	0.55
1:B:346:THR:HB	1:B:351:THR:OG1	2.06	0.55
1:C:462:GLU:CD	1:C:462:GLU:H	2.14	0.55
1:D:129:GLN:HB3	1:D:130:PRO:HD2	1.88	0.55
1:C:306:GLY:C	1:C:308:HIS:H	2.15	0.55
1:D:301:TYR:HD1	1:D:310:GLU:HB2	1.71	0.55
1:A:314:TYR:HB3	1:A:318:ARG:HG3	1.89	0.55
1:A:316:ALA:HB1	1:B:303:TYR:HB3	1.89	0.55
1:A:589:ILE:HD11	1:A:630:ILE:HD13	1.88	0.55
1:D:531:LEU:O	1:D:535:GLU:HG2	2.07	0.55
1:B:192:VAL:HG11	1:B:201:ILE:HD11	1.88	0.55
1:D:609:GLN:NE2	1:D:609:GLN:H	2.04	0.55
1:B:150:PHE:HB2	1:B:449:LEU:HB3	1.88	0.54
1:A:156:PRO:HG3	1:A:279:ARG:NH2	2.21	0.54
1:A:658:GLN:C	1:A:659:LEU:HD12	2.33	0.54
1:D:432:THR:HB	1:D:433:HIS:ND1	2.22	0.54
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.89	0.54
1:C:175:PHE:HD2	1:C:258:ARG:HH11	1.54	0.54
1:B:132:ARG:HB3	1:B:132:ARG:NH1	2.22	0.54
1:A:531:LEU:O	1:A:535:GLU:HG2	2.08	0.54
1:C:326:TYR:CZ	1:C:339:PRO:HB3	2.42	0.54
1:D:332:THR:O	1:D:333:LYS:HB2	2.08	0.54
1:C:444:ALA:HB2	1:C:450:ILE:HD11	1.90	0.54
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.89	0.54
1:B:343:ASN:OD1	1:B:356:TRP:HB2	2.07	0.54
1:B:224:HIS:CE1	1:B:268:THR:HG23	2.43	0.53
1:D:104:ILE:HD12	1:D:104:ILE:H	1.73	0.53
1:C:425:PHE:CE2	1:C:430:ASN:HA	2.43	0.53
1:C:603:SER:HA	1:C:613:VAL:O	2.08	0.53
1:C:388:SER:HB3	1:C:391:ILE:HG12	1.90	0.53
1:D:407:VAL:HG11	1:D:413:ILE:HD11	1.90	0.53
1:C:209:SER:HB2	1:C:224:HIS:HB3	1.91	0.53
1:D:165:TYR:CD1	1:D:189:ARG:HG2	2.44	0.53
1:D:256:PRO:HG3	1:D:266:GLY:N	2.23	0.53
1:D:382:GLY:HA2	1:D:399:LEU:HD11	1.90	0.53
1:D:375:MET:SD	1:D:386:PHE:HB3	2.48	0.53
1:A:323:ASP:OD2	1:B:322:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:PHE:HB2	1:C:648:VAL:HG12	1.91	0.52
1:D:104:ILE:HD12	1:D:104:ILE:N	2.23	0.52
1:D:546:ASN:HB3	1:D:550:ILE:HD13	1.91	0.52
1:D:241:THR:O	1:D:243:THR:HG23	2.09	0.52
1:A:145:GLY:HA3	1:A:452:TYR:CZ	2.44	0.52
1:B:405:SER:HB3	5:B:740:HOH:O	2.08	0.52
1:C:174:TRP:CG	1:C:183:MET:HE2	2.44	0.52
1:C:501:ILE:HG13	1:C:501:ILE:O	2.10	0.52
1:D:248:HIS:HA	1:D:271:CYS:O	2.09	0.52
1:B:265:TYR:HD2	1:B:265:TYR:O	1.92	0.52
1:A:134:PRO:HG2	1:A:526:ILE:HG12	1.90	0.52
1:B:691:ARG:O	1:B:695:LYS:HB2	2.09	0.52
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.91	0.52
1:C:629:ALA:C	1:C:630:ILE:HD12	2.35	0.52
1:B:116:CYS:SG	1:B:622:GLU:HG3	2.49	0.52
1:B:205:GLY:HA3	1:B:328:ARG:NH2	2.25	0.52
1:C:332:THR:C	1:C:334:ALA:H	2.17	0.51
1:D:235:LYS:O	1:D:247:TRP:HA	2.09	0.51
1:C:467:GLU:CD	1:C:470:ARG:HH22	2.18	0.51
1:C:517:VAL:HG13	1:C:518:ASN:N	2.25	0.51
1:D:559:VAL:HG12	1:D:572:THR:HA	1.92	0.51
1:A:198:ILE:O	1:A:203:ALA:HB2	2.11	0.51
1:C:225:ARG:HG2	1:C:254:TYR:CG	2.46	0.51
1:D:658:GLN:C	1:D:659:LEU:HD12	2.36	0.51
1:C:104:ILE:HD12	1:C:104:ILE:H	1.76	0.51
1:D:325:PHE:O	1:D:339:PRO:HA	2.10	0.51
1:A:596:CYS:HB3	1:A:653:TYR:CD2	2.46	0.51
1:A:649:TYR:HB2	1:A:659:LEU:HD11	1.91	0.51
1:C:206:VAL:HG12	1:C:233:GLU:HA	1.92	0.51
1:C:401:GLU:HB3	1:C:442:TYR:CZ	2.46	0.51
1:C:453:GLN:HE21	1:C:454:PRO:HD2	1.76	0.51
1:D:377:ARG:C	1:D:377:ARG:HD2	2.36	0.51
1:C:706:GLN:HB3	1:C:710:GLN:NE2	2.26	0.51
1:D:280:SER:HB2	1:D:287:PHE:HB3	1.93	0.51
1:D:705:VAL:HG12	1:D:709:ASN:HD21	1.76	0.51
1:B:708:ARG:HD3	5:B:5:HOH:O	2.10	0.51
1:D:634:THR:HG22	1:D:635:VAL:H	1.75	0.50
1:A:540:ASN:O	1:A:543:ARG:HG2	2.11	0.50
1:B:255:ASN:HB3	1:B:256:PRO:HD2	1.92	0.50
1:B:301:TYR:HA	1:B:310:GLU:HB2	1.93	0.50
1:A:288:VAL:HG12	1:A:289:LEU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:MET:HG2	1:B:600:PRO:HA	1.92	0.50
1:D:639:ARG:HB3	1:D:641:PHE:CZ	2.46	0.50
1:C:193:PRO:O	1:C:197:VAL:HG23	2.12	0.50
1:C:259:VAL:O	1:C:260:GLU:HB2	2.12	0.50
1:C:377:ARG:HG3	1:C:386:PHE:CE2	2.47	0.50
1:B:125:VAL:N	1:B:568:MET:O	2.45	0.50
1:B:194:PHE:CD1	1:B:320:LYS:HD2	2.46	0.50
1:B:589:ILE:HG22	1:B:592:ARG:H	1.76	0.50
1:C:707:ARG:O	1:C:711:LEU:HB2	2.12	0.50
1:D:366:MET:HE1	1:D:495:ILE:HB	1.93	0.50
1:D:440:GLN:OE1	1:D:471:GLU:HG3	2.12	0.50
1:B:456:LEU:HD21	1:B:461:ALA:HA	1.92	0.50
1:C:346:THR:HA	1:C:351:THR:HA	1.92	0.50
1:A:311:HIS:CG	1:A:312:THR:N	2.79	0.50
1:B:304:ARG:NH1	1:B:341:THR:HG23	2.27	0.49
1:D:250:THR:HG22	1:D:251:ASP:N	2.27	0.49
1:D:397:THR:HG22	1:D:444:ALA:HA	1.92	0.49
1:B:375:MET:SD	1:B:386:PHE:HB3	2.52	0.49
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.11	0.49
1:A:332:THR:C	1:A:334:ALA:H	2.20	0.49
1:B:440:GLN:HE22	1:B:454:PRO:HG3	1.76	0.49
1:D:616:GLN:HG2	1:D:627:ARG:HA	1.93	0.49
1:B:156:PRO:HG2	1:B:279:ARG:NH2	2.27	0.49
1:B:249:THR:HG23	1:B:271:CYS:HB3	1.94	0.49
1:C:147:ALA:HA	1:C:451:ALA:O	2.12	0.49
1:D:199:ASP:O	1:D:203:ALA:HB3	2.13	0.49
1:D:325:PHE:HE2	1:D:327:ALA:HB2	1.77	0.49
1:D:399:LEU:O	1:D:474:ARG:HG3	2.12	0.49
1:B:224:HIS:CD2	1:B:225:ARG:HG3	2.47	0.49
1:B:230:THR:HG22	1:B:231:ASP:H	1.78	0.49
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.13	0.49
1:A:200:LYS:HE3	1:A:208:ARG:NH1	2.28	0.49
1:B:647:TYR:HB2	1:B:659:LEU:HD11	1.94	0.49
1:B:501:ILE:HG13	1:B:501:ILE:O	2.13	0.49
1:B:508:PHE:CE1	1:B:512:HIS:CE1	3.00	0.49
1:D:117:PRO:O	1:D:118:PRO:C	2.56	0.49
1:A:317:ASP:HB2	5:A:739:HOH:O	2.12	0.49
1:A:541:GLU:O	1:A:544:LYS:HB3	2.12	0.49
1:B:196:GLU:O	1:B:200:LYS:HB2	2.13	0.49
1:B:639:ARG:HB3	1:B:641:PHE:CZ	2.47	0.48
1:D:493:GLU:CG	1:D:494:ARG:H	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.95	0.48
1:D:170:VAL:HG23	1:D:265:TYR:CD2	2.48	0.48
1:A:391:ILE:HG22	1:A:393:THR:HG23	1.95	0.48
1:B:116:CYS:HB3	1:B:560:SER:HB3	1.95	0.48
1:D:281:VAL:HG22	1:D:282:TYR:N	2.29	0.48
1:C:557:ARG:HG3	1:C:559:VAL:HG13	1.95	0.48
1:D:129:GLN:HB3	1:D:130:PRO:CD	2.43	0.48
1:B:325:PHE:O	1:B:339:PRO:HA	2.13	0.48
1:D:319:PHE:HB2	1:D:345:LEU:HD13	1.96	0.48
1:A:706:GLN:O	1:A:710:GLN:HG3	2.13	0.48
1:C:104:ILE:HD12	1:C:104:ILE:N	2.28	0.48
1:A:718:ASP:C	1:A:718:ASP:OD1	2.57	0.48
1:C:561:ALA:HB2	1:C:570:VAL:HG12	1.95	0.48
1:D:648:VAL:HG23	1:D:658:GLN:HG2	1.96	0.48
1:B:236:PRO:HA	1:B:247:TRP:CD1	2.49	0.48
1:B:411:ASP:O	1:B:415:LYS:HE2	2.14	0.48
1:C:386:PHE:HB2	1:C:395:PHE:HB2	1.95	0.48
1:D:501:ILE:HG23	1:D:505:ARG:HG3	1.95	0.48
1:A:295:VAL:HG13	1:A:345:LEU:HD23	1.96	0.48
1:B:193:PRO:O	1:B:197:VAL:HG23	2.14	0.48
1:C:191:PRO:HA	1:C:350:PHE:HA	1.96	0.48
1:D:193:PRO:O	1:D:197:VAL:HG23	2.14	0.48
1:D:403:PRO:HG2	1:D:406:ARG:HH21	1.79	0.48
1:A:248:HIS:HA	1:A:271:CYS:O	2.14	0.47
1:C:615:GLY:HA3	1:C:624:ARG:O	2.14	0.47
1:D:192:VAL:HG11	1:D:201:ILE:HD11	1.96	0.47
1:D:222:ALA:HB1	1:D:267:THR:HG21	1.95	0.47
1:A:550:ILE:O	1:A:553:VAL:HG12	2.14	0.47
1:C:147:ALA:HB2	1:C:452:TYR:CD1	2.43	0.47
1:D:175:PHE:HB3	1:D:258:ARG:HE	1.79	0.47
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.79	0.47
1:B:224:HIS:HE1	1:B:268:THR:HG23	1.77	0.47
1:C:106:ALA:HA	1:C:643:PHE:HE2	1.79	0.47
1:D:438:GLN:HB3	1:D:439:PRO:HD2	1.97	0.47
1:D:325:PHE:HB3	1:D:340:THR:O	2.14	0.47
1:A:234:LEU:HD23	1:A:249:THR:HG23	1.96	0.47
1:A:377:ARG:HA	1:A:385:ARG:O	2.14	0.47
1:D:706:GLN:O	1:D:710:GLN:HG3	2.15	0.47
1:B:639:ARG:HB3	1:B:641:PHE:CE1	2.50	0.47
1:C:572:THR:HG22	1:C:573:CYS:N	2.28	0.46
1:D:250:THR:HG22	1:D:252:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.96	0.46
1:B:567:VAL:HG13	1:B:568:MET:N	2.28	0.46
1:B:621:ASN:HD21	1:B:644:GLY:H	1.63	0.46
1:C:513:ILE:O	1:C:514:GLN:C	2.58	0.46
1:D:528:TRP:O	1:D:532:GLN:HG2	2.16	0.46
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.31	0.46
1:C:347:THR:HB	1:C:348:PRO:HD2	1.98	0.46
1:C:599:ARG:HD3	1:C:617:LEU:O	2.16	0.46
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.16	0.46
1:B:192:VAL:HG11	1:B:201:ILE:CD1	2.44	0.46
1:C:626:THR:HG22	1:C:628:ASP:H	1.80	0.46
1:D:114:TYR:HA	1:D:574:VAL:O	2.16	0.46
1:A:119:PRO:HG3	1:A:561:ALA:HA	1.98	0.46
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.96	0.46
1:B:428:ARG:HD3	1:B:429:TYR:CE1	2.51	0.46
1:C:153:ASN:HA	1:C:367:THR:OG1	2.16	0.46
1:D:215:ARG:NH2	1:D:349:LYS:HD3	2.31	0.46
1:B:377:ARG:HA	1:B:385:ARG:O	2.16	0.46
1:B:546:ASN:HB3	1:B:550:ILE:HD13	1.98	0.46
1:D:298:SER:C	1:D:300:PHE:H	2.23	0.46
1:B:224:HIS:C	1:B:226:ASP:H	2.25	0.46
1:C:719:ILE:N	1:C:719:ILE:HD12	2.31	0.46
1:D:300:PHE:O	1:D:307:SER:HB2	2.16	0.45
1:A:402:TYR:HA	1:A:403:PRO:HD3	1.86	0.45
1:B:388:SER:OG	1:B:391:ILE:HG12	2.16	0.45
1:B:607:GLU:H	1:B:607:GLU:HG2	1.53	0.45
1:D:500:SER:OG	1:D:502:GLU:HG2	2.16	0.45
1:C:325:PHE:O	1:C:339:PRO:HA	2.15	0.45
1:D:120:THR:C	1:D:122:ALA:H	2.24	0.45
1:D:209:SER:HB3	1:D:230:THR:H	1.82	0.45
1:D:601:LEU:HD23	1:D:616:GLN:HB3	1.98	0.45
1:C:209:SER:HB2	1:C:224:HIS:CB	2.47	0.45
1:C:259:VAL:HG23	1:C:260:GLU:CD	2.42	0.45
1:A:397:THR:HG22	1:A:398:ASN:N	2.32	0.45
1:D:115:VAL:O	1:D:117:PRO:HD3	2.17	0.45
1:D:250:THR:HG22	1:D:251:ASP:H	1.82	0.45
1:A:188:ASP:OD1	1:A:215:ARG:NH2	2.48	0.45
1:B:248:HIS:HB2	1:B:270:ASN:OD1	2.17	0.45
1:B:365:THR:O	1:B:366:MET:HE2	2.16	0.45
1:D:301:TYR:HA	1:D:307:SER:O	2.17	0.45
1:B:174:TRP:C	1:B:174:TRP:CD1	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLU:HB2	1:B:296:TYR:HA	1.99	0.45
1:A:649:TYR:O	1:A:656:SER:HB3	2.16	0.45
1:C:550:ILE:O	1:C:553:VAL:HG12	2.17	0.45
1:D:252:LEU:HD12	1:D:252:LEU:N	2.31	0.45
1:D:265:TYR:CD2	1:D:265:TYR:C	2.95	0.45
1:B:113:PHE:O	1:B:575:PRO:HA	2.16	0.45
1:B:597:TYR:CE1	1:B:601:LEU:HD11	2.52	0.45
1:C:512:HIS:CE1	1:C:515:ARG:HH22	2.34	0.45
1:C:589:ILE:HG12	1:C:597:TYR:CE1	2.52	0.45
1:D:515:ARG:O	1:D:519:ASP:HB2	2.17	0.45
1:B:201:ILE:HG23	1:B:234:LEU:CD1	2.47	0.44
1:B:358:PRO:HB2	1:B:361:PRO:HD2	1.99	0.44
1:B:304:ARG:HH11	1:B:341:THR:CG2	2.28	0.44
1:C:468:HIS:CD2	1:C:468:HIS:C	2.95	0.44
1:C:564:LEU:HD11	1:C:569:ALA:HB2	2.00	0.44
1:D:444:ALA:HB3	1:D:448:PHE:HB2	1.98	0.44
1:C:421:MET:SD	1:C:453:GLN:HB2	2.57	0.44
1:D:166:LYS:HE2	1:D:207:CYS:SG	2.57	0.44
1:D:165:TYR:HA	1:D:192:VAL:HG23	1.99	0.44
1:D:506:LEU:O	1:D:507:GLN:C	2.61	0.44
1:A:392:SER:HA	1:A:508:PHE:CE2	2.52	0.44
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.99	0.44
1:D:301:TYR:CD1	1:D:310:GLU:HB2	2.52	0.44
1:D:412:CYS:O	1:D:413:ILE:C	2.60	0.44
1:B:440:GLN:OE1	1:B:454:PRO:HG2	2.17	0.44
1:C:343:ASN:C	1:C:344:LEU:HG	2.43	0.44
1:D:603:SER:HA	1:D:613:VAL:O	2.18	0.44
1:D:152:GLU:HA	1:D:366:MET:SD	2.58	0.44
1:D:366:MET:CE	1:D:495:ILE:HB	2.48	0.44
1:A:354:TRP:N	1:A:354:TRP:CE3	2.86	0.44
1:C:552:SER:HA	1:C:559:VAL:HG22	1.99	0.44
1:B:162:THR:HA	1:B:274:GLU:O	2.18	0.43
1:B:175:PHE:CG	1:B:258:ARG:HB3	2.53	0.43
1:B:179:TYR:CD1	1:B:179:TYR:C	2.96	0.43
1:C:401:GLU:HG2	1:C:474:ARG:O	2.17	0.43
1:C:719:ILE:HD12	1:C:719:ILE:H	1.83	0.43
1:B:263:HIS:NE2	1:B:265:TYR:CE2	2.86	0.43
1:B:475:LYS:HA	1:B:476:PRO:HD3	1.87	0.43
1:C:318:ARG:O	1:C:346:THR:HG22	2.18	0.43
1:D:125:VAL:HG22	1:D:568:MET:O	2.18	0.43
1:B:400:THR:O	1:B:442:TYR:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:THR:HG22	1:B:498:THR:O	2.18	0.43
1:A:440:GLN:O	1:A:451:ALA:HA	2.19	0.43
1:A:515:ARG:HD2	5:A:750:HOH:O	2.18	0.43
1:D:155:ALA:HA	1:D:156:PRO:HD3	1.85	0.43
1:A:151:LYS:O	1:A:152:GLU:C	2.61	0.43
1:B:200:LYS:HE3	1:B:208:ARG:CZ	2.48	0.43
1:B:332:THR:O	1:B:333:LYS:HB2	2.19	0.43
1:C:106:ALA:HA	1:C:643:PHE:CE2	2.53	0.43
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.87	0.43
1:A:347:THR:HB	1:A:348:PRO:HD2	2.00	0.43
1:A:391:ILE:HG22	1:A:391:ILE:O	2.18	0.43
1:B:302:GLY:O	1:B:308:HIS:HA	2.19	0.43
1:C:402:TYR:CD1	1:C:403:PRO:HD2	2.53	0.43
1:D:343:ASN:C	1:D:344:LEU:HD12	2.44	0.43
1:D:420:ALA:HA	1:D:423:ARG:CZ	2.48	0.43
1:A:377:ARG:HH21	1:A:454:PRO:HG3	1.83	0.43
1:A:690:THR:OG1	1:A:693:GLU:HG3	2.19	0.43
1:B:132:ARG:HB3	1:B:132:ARG:HH11	1.84	0.43
1:C:673:LEU:HG	1:C:675:ILE:HG12	2.01	0.43
1:B:318:ARG:O	1:B:345:LEU:HA	2.19	0.43
1:A:105:LYS:O	1:A:658:GLN:NE2	2.52	0.43
1:A:440:GLN:HE22	1:A:471:GLU:HB3	1.84	0.43
1:C:332:THR:C	1:C:334:ALA:N	2.77	0.43
1:D:319:PHE:CZ	1:D:321:GLN:HB2	2.54	0.43
1:C:464:TYR:C	1:C:464:TYR:CD2	2.96	0.43
1:B:230:THR:CG2	1:B:231:ASP:N	2.82	0.42
1:B:466:ARG:HH22	1:B:470:ARG:HB2	1.83	0.42
1:C:360:ARG:HB2	1:C:361:PRO:HD3	2.01	0.42
1:A:403:PRO:HB2	1:A:406:ARG:HB2	2.01	0.42
1:B:341:THR:HB	1:B:356:TRP:HB3	2.01	0.42
1:B:468:HIS:C	1:B:468:HIS:CD2	2.97	0.42
1:B:718:ASP:HB3	1:B:721:THR:HG23	2.01	0.42
1:C:436:VAL:HB	1:C:454:PRO:HB2	2.02	0.42
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.80	0.42
1:B:329:ASP:HB3	1:B:332:THR:OG1	2.20	0.42
1:B:585:ASN:OD1	1:B:585:ASN:N	2.50	0.42
1:C:129:GLN:HB3	1:C:130:PRO:HD2	2.01	0.42
1:C:630:ILE:CG2	1:C:631:GLU:N	2.82	0.42
1:C:634:THR:HB	1:C:637:HIS:HB2	2.01	0.42
1:D:190:ALA:HA	1:D:191:PRO:HD3	1.87	0.42
1:A:298:SER:HB3	1:A:310:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LYS:HA	1:A:476:PRO:HD3	1.90	0.42
1:C:464:TYR:C	1:C:464:TYR:HD2	2.26	0.42
1:C:519:ASP:O	1:C:523:ARG:HG3	2.19	0.42
1:C:634:THR:O	1:C:653:TYR:HE1	2.03	0.42
1:D:147:ALA:HA	1:D:451:ALA:O	2.19	0.42
1:D:511:ASN:O	1:D:512:HIS:C	2.62	0.42
1:D:659:LEU:HD12	1:D:659:LEU:N	2.35	0.42
1:C:256:PRO:HD3	1:C:266:GLY:HA3	2.01	0.42
1:C:344:LEU:HA	1:C:352:VAL:O	2.19	0.42
1:D:328:ARG:HH12	1:D:335:ARG:HB2	1.84	0.42
1:B:140:GLN:HB3	1:B:142:TYR:CE1	2.55	0.42
1:D:255:ASN:HA	1:D:256:PRO:HD3	1.82	0.42
1:D:439:PRO:HD3	1:D:453:GLN:OE1	2.19	0.42
1:B:366:MET:CE	1:B:495:ILE:HB	2.50	0.42
1:C:396:THR:O	1:C:444:ALA:HA	2.19	0.42
1:D:201:ILE:O	1:D:205:GLY:HA2	2.19	0.42
1:D:442:TYR:O	1:D:449:LEU:HD12	2.20	0.42
1:A:596:CYS:HB3	1:A:653:TYR:CE2	2.55	0.42
1:C:325:PHE:HB3	1:C:340:THR:O	2.19	0.42
1:D:171:SER:O	1:D:265:TYR:HB2	2.20	0.42
1:D:522:GLY:O	1:D:526:ILE:HG13	2.20	0.42
1:A:150:PHE:HB3	1:A:366:MET:HE3	2.02	0.42
1:A:191:PRO:O	1:A:192:VAL:C	2.61	0.42
1:A:240:ALA:HB3	1:A:243:THR:HG21	2.01	0.42
1:A:248:HIS:HE1	1:A:251:ASP:OD2	2.02	0.42
1:A:545:LEU:O	1:A:547:PRO:HD3	2.20	0.42
1:B:621:ASN:OD1	1:B:643:PHE:HA	2.20	0.42
1:D:282:TYR:CG	1:D:283:PRO:HA	2.55	0.42
1:D:536:LEU:O	1:D:537:THR:C	2.63	0.42
1:B:621:ASN:ND2	1:B:644:GLY:H	2.18	0.41
1:D:402:TYR:HA	1:D:403:PRO:HD3	1.87	0.41
1:C:420:ALA:HA	1:C:423:ARG:NH2	2.34	0.41
1:C:526:ILE:O	1:C:530:GLU:HG3	2.20	0.41
1:C:125:VAL:O	1:C:567:VAL:HG22	2.20	0.41
1:C:163:MET:O	1:C:273:VAL:HG13	2.19	0.41
1:C:517:VAL:HG13	1:C:518:ASN:H	1.83	0.41
1:D:201:ILE:HG12	1:D:206:VAL:O	2.20	0.41
1:B:655:TYR:CD2	1:B:655:TYR:C	2.99	0.41
1:D:114:TYR:HB3	1:D:573:CYS:HB3	2.03	0.41
1:D:323:ASP:OD1	1:D:341:THR:HG22	2.20	0.41
1:A:512:HIS:CE1	1:A:515:ARG:HH12	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ALA:HA	1:B:451:ALA:O	2.20	0.41
1:D:209:SER:OG	1:D:224:HIS:HB3	2.21	0.41
1:B:281:VAL:O	1:B:282:TYR:C	2.63	0.41
1:C:555:VAL:HG13	1:C:557:ARG:HG2	2.02	0.41
1:C:722:VAL:C	1:C:723:ILE:HD12	2.45	0.41
1:D:174:TRP:HZ3	1:D:179:TYR:HH	1.67	0.41
1:D:502:GLU:HG3	1:D:503:PHE:H	1.85	0.41
1:A:120:THR:C	1:A:122:ALA:H	2.29	0.41
1:D:326:TYR:HD1	1:D:336:ALA:O	2.03	0.41
1:B:129:GLN:HB3	1:B:130:PRO:CD	2.51	0.41
1:C:675:ILE:HD13	1:C:675:ILE:HA	1.95	0.41
1:A:520:MET:HE1	1:A:523:ARG:NH2	2.36	0.41
1:A:587:MET:HG3	1:A:650:PHE:CE2	2.55	0.41
1:A:701:ASP:O	1:A:702:TYR:C	2.64	0.41
1:B:190:ALA:HA	1:B:191:PRO:HD3	1.83	0.41
1:B:194:PHE:CD2	1:B:320:LYS:HD2	2.55	0.41
1:B:244:SER:O	3:B:4000:MRY:HAE	2.20	0.41
1:C:377:ARG:HB3	1:C:377:ARG:HH11	1.86	0.41
1:C:401:GLU:OE1	1:C:440:GLN:HB2	2.21	0.41
1:C:467:GLU:O	1:C:471:GLU:HG2	2.20	0.41
1:D:346:THR:HG22	1:D:351:THR:HG23	2.03	0.41
1:A:106:ALA:HA	1:A:643:PHE:CE2	2.56	0.41
1:A:561:ALA:HB2	1:A:570:VAL:HG12	2.03	0.41
1:B:163:MET:O	1:B:273:VAL:HA	2.21	0.41
1:C:506:LEU:O	1:C:507:GLN:C	2.64	0.41
1:D:191:PRO:HA	1:D:350:PHE:HA	2.02	0.41
1:D:298:SER:HA	1:D:299:PRO:HD3	1.91	0.41
1:D:473:SER:C	1:D:475:LYS:H	2.29	0.41
1:A:285:ASP:HB2	1:A:311:HIS:HB3	2.03	0.40
1:B:397:THR:HG22	1:B:444:ALA:HA	2.01	0.40
1:B:546:ASN:O	1:B:547:PRO:C	2.64	0.40
1:B:588:ARG:HA	1:B:596:CYS:SG	2.60	0.40
1:C:155:ALA:HA	1:C:156:PRO:HD3	1.92	0.40
1:D:236:PRO:HA	1:D:247:TRP:CD1	2.55	0.40
1:A:311:HIS:CD2	1:A:312:THR:N	2.89	0.40
1:A:497:THR:HG22	1:A:498:THR:O	2.21	0.40
1:C:104:ILE:O	1:C:582:ILE:HG23	2.21	0.40
1:A:520:MET:HE1	1:A:523:ARG:HH21	1.85	0.40
1:A:601:LEU:HD23	1:A:627:ARG:CD	2.49	0.40
1:B:157:TYR:CE2	1:B:159:PHE:CD2	3.09	0.40
1:C:192:VAL:HG11	1:C:201:ILE:CD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:VAL:O	1:D:201:ILE:HB	2.22	0.40
1:D:426:ALA:O	1:D:430:ASN:HB2	2.20	0.40
1:A:163:MET:SD	1:A:289:LEU:HD13	2.62	0.40
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.90	0.40
1:C:536:LEU:O	1:C:537:THR:C	2.63	0.40
1:A:591:SER:C	1:A:593:PRO:HD3	2.46	0.40
1:B:156:PRO:O	1:B:158:LYS:HD2	2.22	0.40
1:C:347:THR:N	1:C:350:PHE:O	2.54	0.40
1:D:386:PHE:HB2	1:D:395:PHE:HB2	2.04	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	599/703 (85%)	544 (91%)	51 (8%)	4 (1%)	18	53
1	B	591/703 (84%)	543 (92%)	47 (8%)	1 (0%)	43	76
1	C	597/703 (85%)	543 (91%)	52 (9%)	2 (0%)	36	70
1	D	599/703 (85%)	535 (89%)	61 (10%)	3 (0%)	24	60
All	All	2386/2812 (85%)	2165 (91%)	211 (9%)	10 (0%)	30	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	SER
1	C	237	ALA
1	D	199	ASP
1	A	413	ILE
1	A	688	VAL
1	D	198	ILE

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Mol	Chain	Res	Type
1	A	517	VAL
1	D	134	PRO
1	A	324	GLY
1	C	413	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/593 (86%)	493 (96%)	19 (4%)	30	64
1	B	507/593 (86%)	481 (95%)	26 (5%)	21	55
1	C	494/593 (83%)	473 (96%)	21 (4%)	26	60
1	D	511/593 (86%)	481 (94%)	30 (6%)	18	50
All	All	2024/2372 (85%)	1928 (95%)	96 (5%)	23	58

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	140	GLN
1	A	227	ASP
1	A	230	THR
1	A	235	LYS
1	A	250	THR
1	A	258	ARG
1	A	259	VAL
1	A	263	HIS
1	A	309	THR
1	A	337	THR
1	A	387	SER
1	A	404	LEU
1	A	463	LEU
1	A	469	LEU
1	A	492	VAL
1	A	502	GLU

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Mol	Chain	Res	Type
1	A	584	GLN
1	A	679	GLU
1	B	124	VAL
1	B	125	VAL
1	B	177	HIS
1	B	181	GLN
1	B	255	ASN
1	B	265	TYR
1	B	267	THR
1	B	323	ASP
1	B	329	ASP
1	B	346	THR
1	B	363	VAL
1	B	377	ARG
1	B	389	ASP
1	B	401	GLU
1	B	434	ILE
1	B	440	GLN
1	B	469	LEU
1	B	492	VAL
1	B	585	ASN
1	B	607	GLU
1	B	626	THR
1	B	635	VAL
1	B	659	LEU
1	B	676	THR
1	B	679	GLU
1	B	721	THR
1	C	108	ASN
1	C	112	ASN
1	C	120	THR
1	C	189	ARG
1	C	241	THR
1	C	250	THR
1	C	258	ARG
1	C	267	THR
1	C	271	CYS
1	C	346	THR
1	C	377	ARG
1	C	392	SER
1	C	530	GLU
1	C	546	ASN

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Mol	Chain	Res	Type
1	C	567	VAL
1	C	584	GLN
1	C	660	SER
1	C	679	GLU
1	C	711	LEU
1	C	719	ILE
1	C	722	VAL
1	D	140	GLN
1	D	170	VAL
1	D	173	VAL
1	D	179	TYR
1	D	189	ARG
1	D	228	HIS
1	D	241	THR
1	D	252	LEU
1	D	308	HIS
1	D	311	HIS
1	D	313	SER
1	D	323	ASP
1	D	365	THR
1	D	368	LYS
1	D	389	ASP
1	D	401	GLU
1	D	409	LEU
1	D	412	CYS
1	D	470	ARG
1	D	471	GLU
1	D	494	ARG
1	D	500	SER
1	D	501	ILE
1	D	502	GLU
1	D	558	ARG
1	D	609	GLN
1	D	634	THR
1	D	635	VAL
1	D	648	VAL
1	D	721	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS

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Mol	Chain	Res	Type
1	A	512	HIS
1	A	532	GLN
1	B	433	HIS
1	B	468	HIS
1	B	512	HIS
1	C	321	GLN
1	C	621	ASN
1	C	709	ASN
1	C	710	GLN
1	D	129	GLN
1	D	140	GLN
1	D	181	GLN
1	D	224	HIS
1	D	445	ASN
1	D	511	ASN
1	D	609	GLN
1	D	692	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1141	1	14,14,15	0.50	0	17,19,21	1.15	1 (5%)
2	NAG	D	1141	1	14,14,15	0.51	0	17,19,21	0.74	0
2	NAG	C	1398	1	14,14,15	0.48	0	17,19,21	0.82	1 (5%)
2	NAG	C	1674	1	14,14,15	0.49	0	17,19,21	0.76	0
3	MRY	A	4000	-	7,7,7	0.59	0	8,8,8	0.95	0
2	NAG	B	1430	1	14,14,15	0.64	0	17,19,21	0.98	1 (5%)
3	MRY	B	4000	-	7,7,7	0.63	0	8,8,8	0.86	0
2	NAG	A	1674	1	14,14,15	0.47	0	17,19,21	0.83	0
2	NAG	A	1398	1	14,14,15	0.57	0	17,19,21	0.73	0
2	NAG	C	1141	1	14,14,15	0.52	0	17,19,21	0.89	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1141	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1398	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
3	MRY	A	4000	-	-	0/8/8/8	-
2	NAG	B	1430	1	-	1/6/23/26	0/1/1/1
3	MRY	B	4000	-	-	0/8/8/8	-
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1398	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1141	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(°)	Ideal(°)
2	A	1141	NAG	C1-O5-C5	3.05	116.27	112.19
2	B	1430	NAG	C1-O5-C5	2.39	115.39	112.19
2	C	1141	NAG	C1-O5-C5	2.38	115.38	112.19
2	C	1398	NAG	C1-O5-C5	2.12	115.03	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1430	NAG	C1-C2-N2-C7
2	A	1398	NAG	C4-C5-C6-O6
2	A	1398	NAG	O5-C5-C6-O6
2	C	1398	NAG	O5-C5-C6-O6
2	D	1141	NAG	O5-C5-C6-O6
2	C	1398	NAG	C1-C2-N2-C7
2	A	1398	NAG	C8-C7-N2-C2
2	A	1398	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1141	NAG	1	0
3	B	4000	MRY	3	0
2	A	1398	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	605/703 (86%)	-1.67	0 100 100	5, 46, 115, 474	0
1	B	596/703 (84%)	-1.64	0 100 100	9, 53, 129, 232	1 (0%)
1	C	603/703 (85%)	-1.53	0 100 100	19, 72, 139, 454	0
1	D	605/703 (86%)	-1.59	0 100 100	17, 62, 124, 292	0
All	All	2409/2812 (85%)	-1.61	0 100 100	5, 59, 129, 474	1 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	NAG	B	1430	14/15	0.97	0.04	85,85,85,85	0
2	NAG	C	1141	14/15	0.98	0.04	113,113,113,113	0
2	NAG	C	1674	14/15	0.98	0.03	87,87,87,87	0
2	NAG	D	1141	14/15	0.98	0.04	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1674	14/15	0.99	0.03	73,73,73,73	0
2	NAG	C	1398	14/15	0.99	0.03	94,94,94,94	0
2	NAG	A	1141	14/15	0.99	0.03	81,81,81,81	0
2	NAG	A	1398	14/15	0.99	0.03	52,58,58,58	0
3	MRY	A	4000	8/8	0.99	0.04	54,54,54,54	0
3	MRY	B	4000	8/8	0.99	0.03	47,47,47,47	0
4	NA	A	751	1/1	0.99	0.07	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.