Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID	:	3NWF
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

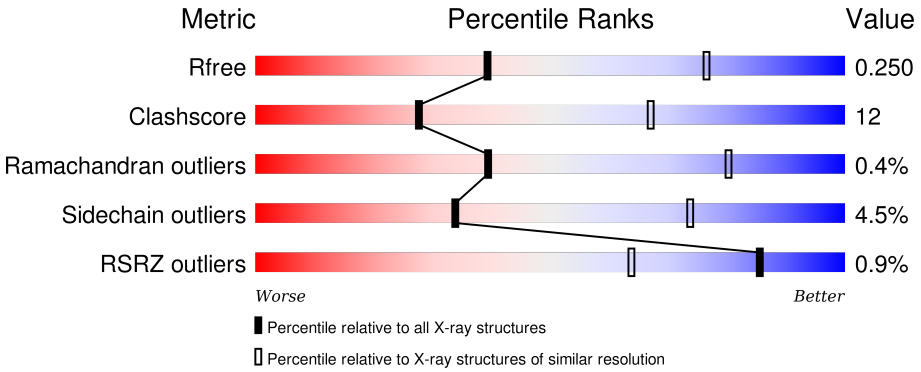
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	703	% 64% 22% 14%
1	B	703	% 60% 23% • 15%
1	C	703	% 60% 24% • 14%
1	D	703	% 59% 24% • 14%

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
3	MRY	A	4000	-	-	-	X

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.

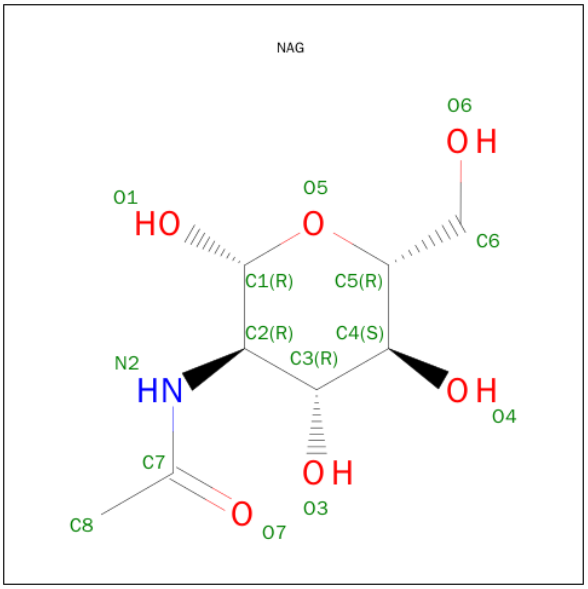
- Molecule 1 is a protein called Envelope glycoprotein B.

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:

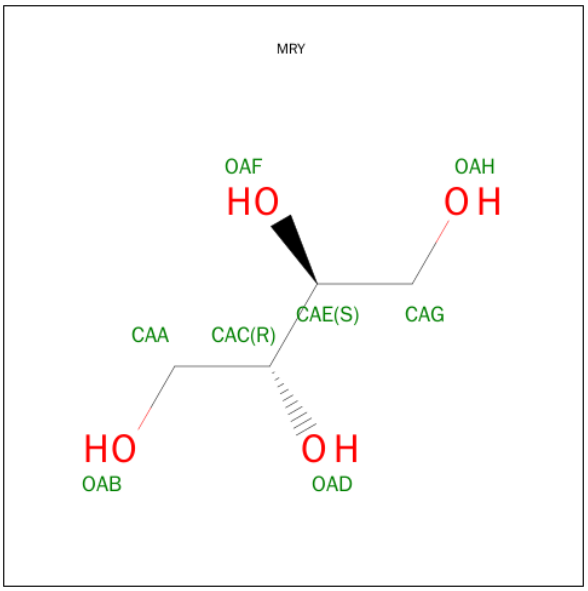
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	EXPRESSION TAG	UNP P06437
B	29	PRO	-	EXPRESSION TAG	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	EXPRESSION TAG	UNP P06437
A	29	PRO	-	EXPRESSION TAG	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	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	A	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 (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

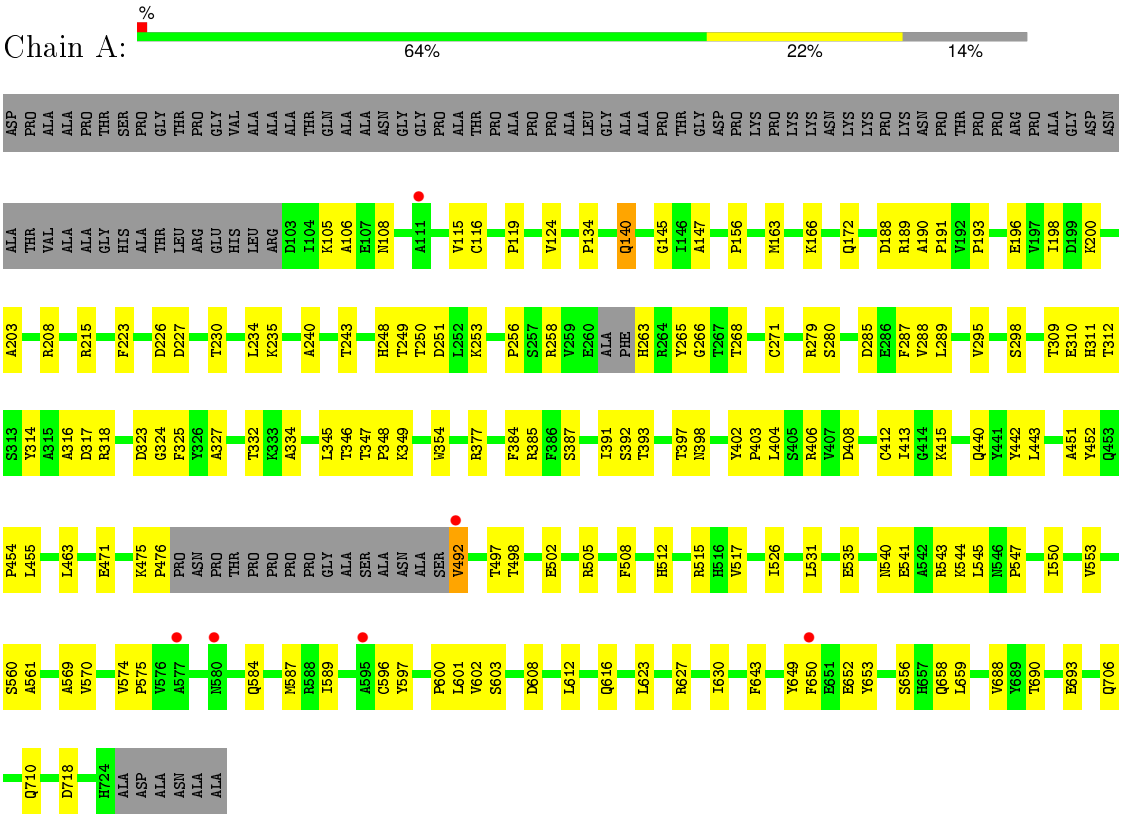
- Molecule 5 is water.

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

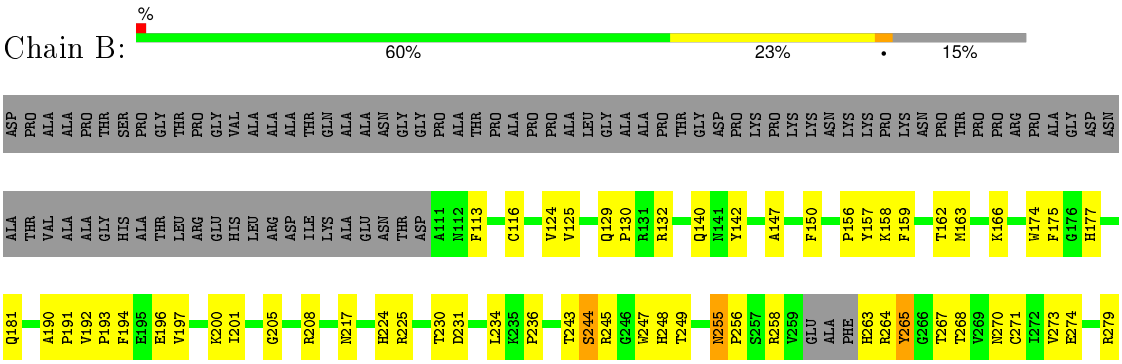
3 Residue-property plots (i)

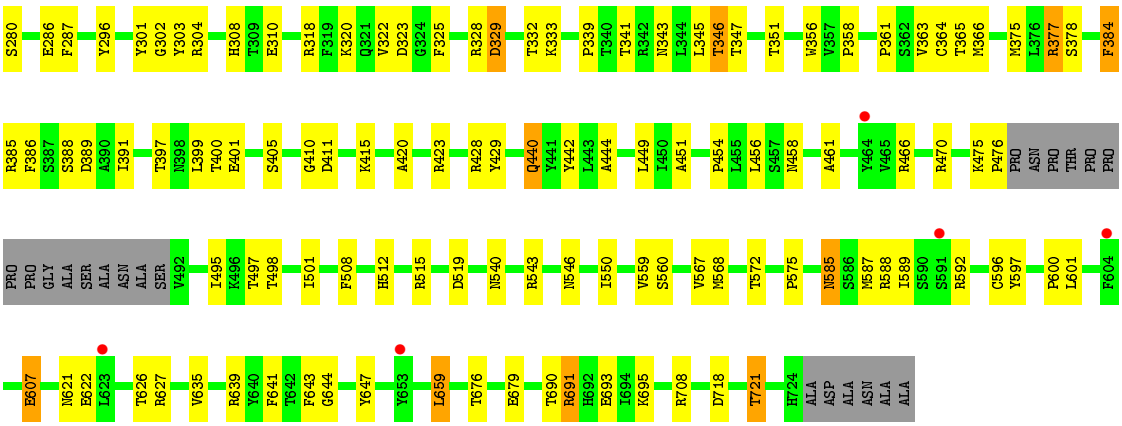
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Envelope glycoprotein B



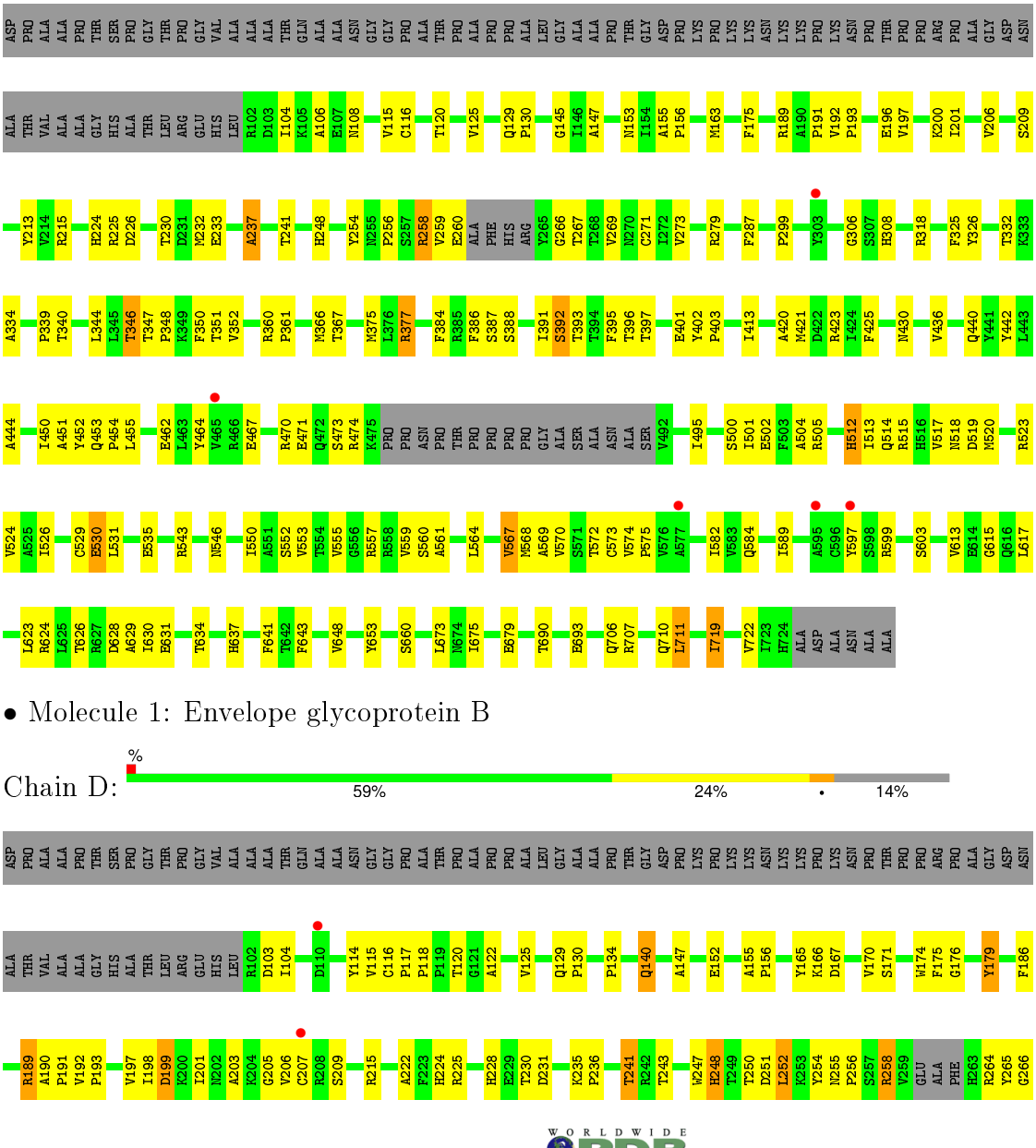
- Molecule 1: Envelope glycoprotein B





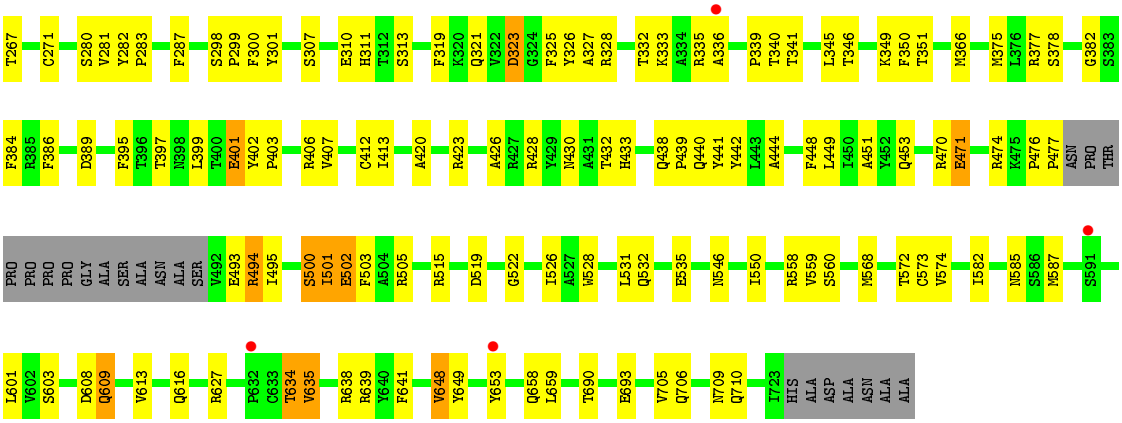
• Molecule 1: Envelope glycoprotein B

Chain C:



• Molecule 1: Envelope glycoprotein B

Chain D:


T267 C271 S280 V281 Y282 P283 F287 S298 P299 F300 Y301 S307 E310 H311 T312 S313 F319 K320 Q321 Y322 D323 G324 F325 Y326 A327 R328 T332 K333 A334 R335 A336 P339 T340 T341 L345 T346 K349 F350 T351 M366 M375 L376 R377 S378 G382 S383
F384 R385 F386 D389 F395 T396 T397 N398 L399 T400 E401 Y402 P403 R406 V407 C412 I413 A420 R423 A426 R427 R428 Y429 N430 A431 T432 H433 Q438 P439 Q440 Y441 Y442 L443 A444 F448 L449 I450 A451 Y452 Q453 R470 E471 R474 K475 P476 P477 ASN PRO THR
PRO PRO PRO PRO GLY ALA SER ALA ASN ALA SER V492 E493 R494 I495 S500 I501 E502 F503 A504 R505 R515 D519 G522 I526 A527 W528 L531 Q532 E535 N546 I550 R558 V559 S560 M568 T572 C573 V574 I582 N585 S586 M587 S591
L601 V602 S603 D608 Q609 V613 Q616 R627 P632 G633 T634 V635 R638 R639 Y640 F641 V648 Y649 Y653 Q658 L659 T690 E693 V705 Q706 N709 Q710 V723 HIS ALA ASP ALA ASN ALA ALA

4 Data and refinement statistics (i)

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 50.37 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.54-3.00) 86.6 (50.37-2.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 0.250	Depositor DCC
R_{free} test set	4528 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.7	EDS
Estimated twinning fraction	0.038 for -h,-k,l 0.460 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 112550 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[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: NA, NAG, MRY

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	0.25	0/4931	0.43	0/6708
1	B	0.24	0/4884	0.42	0/6644
1	C	0.23	0/4840	0.41	0/6599
1	D	0.24	0/4930	0.42	0/6713
All	All	0.24	0/19585	0.42	0/26664

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4814	0	4593	89	0
1	B	4762	0	4552	115	0
1	C	4727	0	4425	116	0
1	D	4813	0	4565	126	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	444	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 12.

All (444) 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: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:265:TYR:HD2	1:B:265:TYR:C	1.92	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: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:D:140:GLN:NE2	1:D:378:SER:HB2	2.07	0.66
1:B:265:TYR:CD2	1:B:265:TYR:C	2.67	0.66
1:A:166:LYS:HB2	1:A:190:ALA:HB3	1.77	0.66
1:D:176:GLY:HA3	1:D:179:TYR:CE1	2.29	0.65
1:B:194:PHE:CG	1:B:320:LYS:HD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:CYS:HB3	1:D:560:SER:HB3	1.77	0.65
1:D:401:GLU:HB2	1:D:474:ARG:O	1.96	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:D:587:MET:HE2	1:D:653:TYR:HA	1.78	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:B:567:VAL:HG22	1:B:568:MET:H	1.63	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:679:GLU:H	1:C:679:GLU:CD	2.02	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: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:A:443:LEU:O	2:A:1398:NAG:H81	2.01	0.60
1:A:408:ASP:HB2	1:A:492:VAL:HG13	1.84	0.60
1:D:103:ASP:HB3	1:D:582:ILE:HD13	1.83	0.60
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:A:603:SER:HB3	1:A:612:LEU:HD21	1.85	0.59
1:C:520:MET:O	1:C:524:VAL:HG23	2.01	0.59
1:B:304:ARG:HH11	1:B:341:THR:HG23	1.68	0.59
1:A:253:LYS:HD3	1:A:268:THR:HG21	1.84	0.59
1:D:401:GLU:HG2	1:D:441:TYR:O	2.02	0.59
1:C:287:PHE:HB3	1:C:299:PRO:HG3	1.85	0.59
1:C:259:VAL:HG23	1:C:260:GLU:OE1	2.03	0.59
1:B:201:ILE:O	1:B:205:GLY:HA2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:142:TYR:CD2	1:B:378:SER:HB3	2.38	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:C:393:THR:HG23	1:C:504:ALA:HB1	1.87	0.56
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:B:245:ARG:HA	3:B:4000:MRY:HAG2	1.87	0.56
1:B:166:LYS:HG2	1:B:271:CYS:HA	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
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:D:384:PHE:CE2	1:D:399:LEU:HA	2.41	0.55
1:B:384:PHE:CE2	1:B:399:LEU:HA	2.41	0.55
1:D:420:ALA:HA	1:D:423:ARG:NH2	2.21	0.55
1:D:129:GLN:HB3	1:D:130:PRO:HD2	1.88	0.55
1:B:346:THR:HB	1:B:351:THR:OG1	2.06	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:H	1:D:609:GLN:NE2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:432:THR:HB	1:D:433:HIS:ND1	2.22	0.54
1:C:175:PHE:HD2	1:C:258:ARG:HH11	1.54	0.54
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.89	0.54
1:B:132:ARG:NH1	1:B:132:ARG:HB3	2.22	0.54
1:C:326:TYR:CZ	1:C:339:PRO:HB3	2.42	0.54
1:A:531:LEU:O	1:A:535:GLU:HG2	2.08	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:B:343:ASN:OD1	1:B:356:TRP:HB2	2.07	0.54
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.89	0.54
1:B:224:HIS:CE1	1:B:268:THR:HG23	2.43	0.53
1:D:104:ILE:H	1:D:104:ILE:HD12	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:C:375:MET:HE1	1:C:388:SER:HB2	1.91	0.53
1:D:407:VAL:HG11	1:D:413:ILE:HD11	1.90	0.53
1:D:165:TYR:CD1	1:D:189:ARG:HG2	2.44	0.53
1:C:209:SER:HB2	1:C:224:HIS:HB3	1.91	0.53
1:D:382:GLY:HA2	1:D:399:LEU:HD11	1.90	0.53
1:D:256:PRO:HG3	1:D:266:GLY:N	2.23	0.53
1:D:375:MET:SD	1:D:386:PHE:HB3	2.48	0.53
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:C:641:PHE:HB2	1:C:648:VAL:HG12	1.91	0.52
1:A:323:ASP:OD2	1:B:322:VAL:HG13	2.09	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:D:248:HIS:HA	1:D:271:CYS:O	2.09	0.52
1:C:501:ILE:O	1:C:501:ILE:HG13	2.10	0.52
1:B:265:TYR:HD2	1:B:265:TYR:O	1.92	0.52
1:B:691:ARG:O	1:B:695:LYS:HB2	2.09	0.52
1:A:134:PRO:HG2	1:A:526:ILE:HG12	1.90	0.52
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.91	0.52
1:B:205:GLY:HA3	1:B:328:ARG:NH2	2.25	0.52
1:B:116:CYS:SG	1:B:622:GLU:HG3	2.49	0.52
1:D:235:LYS:O	1:D:247:TRP:HA	2.09	0.51
1:C:517:VAL:HG13	1:C:518:ASN:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:559:VAL:HG12	1:D:572:THR:HA	1.92	0.51
1:C:225:ARG:HG2	1:C:254:TYR:CG	2.46	0.51
1:A:198:ILE:O	1:A:203:ALA:HB2	2.11	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:C:401:GLU:HB3	1:C:442:TYR:CZ	2.46	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:453:GLN:HE21	1:C:454:PRO:HD2	1.76	0.51
1:C:206:VAL:HG12	1:C:233:GLU:HA	1.92	0.51
1:D:705:VAL:HG12	1:D:709:ASN:HD21	1.76	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: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:C:462:GLU:CD	1:C:462:GLU:H	2.14	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
1:D:639:ARG:HB3	1:D:641:PHE:CZ	2.46	0.50
1:B:587:MET:HG2	1:B:600:PRO:HA	1.92	0.50
1:C:306:GLY:C	1:C:308:HIS:H	2.15	0.50
1:C:259:VAL:O	1:C:260:GLU:HB2	2.12	0.50
1:C:193:PRO:O	1:C:197:VAL:HG23	2.12	0.50
1:C:377:ARG:HG3	1:C:386:PHE:CE2	2.47	0.50
1:B:194:PHE:CD1	1:B:320:LYS:HD2	2.46	0.50
1:B:125:VAL:N	1:B:568:MET:O	2.45	0.50
1:C:707:ARG:O	1:C:711:LEU:HB2	2.12	0.50
1:B:589:ILE:HG22	1:B:592:ARG:H	1.76	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:A:658:GLN:C	1:A:659:LEU:HD12	2.33	0.50
1:B:304:ARG:NH1	1:B:341:THR:HG23	2.27	0.49
1:D:397:THR:HG22	1:D:444:ALA:HA	1.92	0.49
1:D:250:THR:HG22	1:D:251:ASP:N	2.27	0.49
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.11	0.49
1:B:375:MET:SD	1:B:386:PHE:HB3	2.52	0.49
1:B:440:GLN:HE22	1:B:454:PRO:HG3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:GLN:HG2	1:D:627:ARG:HA	1.93	0.49
1:C:147:ALA:HA	1:C:451:ALA:O	2.12	0.49
1:D:399:LEU:O	1:D:474:ARG:HG3	2.12	0.49
1:B:249:THR:HG23	1:B:271:CYS:HB3	1.94	0.49
1:D:325:PHE:HE2	1:D:327:ALA:HB2	1.77	0.49
1:D:199:ASP:O	1:D:203:ALA:HB3	2.13	0.49
1:B:156:PRO:HG2	1:B:279:ARG:NH2	2.27	0.49
1:B:230:THR:HG22	1:B:231:ASP:H	1.78	0.49
1:B:224:HIS:CD2	1:B:225:ARG:HG3	2.47	0.49
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.13	0.49
1:B:647:TYR:HB2	1:B:659:LEU:HD11	1.94	0.49
1:A:200:LYS:HE3	1:A:208:ARG:NH1	2.28	0.49
1:B:501:ILE:O	1:B:501:ILE:HG13	2.13	0.49
1:B:508:PHE:CE1	1:B:512:HIS:CE1	3.00	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:A:317:ASP:HB2	5:A:739:HOH:O	2.12	0.49
1:D:493:GLU:CG	1:D:494:ARG:H	2.24	0.48
1:B:639:ARG:HB3	1:B:641:PHE:CZ	2.47	0.48
1:D:170:VAL:HG23	1:D:265:TYR:CD2	2.48	0.48
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.95	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:D:129:GLN:HB3	1:D:130:PRO:CD	2.43	0.48
1:C:557:ARG:HG3	1:C:559:VAL:HG13	1.95	0.48
1:D:319:PHE:HB2	1:D:345:LEU:HD13	1.96	0.48
1:B:325:PHE:O	1:B:339:PRO:HA	2.13	0.48
1:C:104:ILE:HD12	1:C:104:ILE:N	2.28	0.48
1:A:706:GLN:O	1:A:710:GLN:HG3	2.13	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:C:386:PHE:HB2	1:C:395:PHE:HB2	1.95	0.48
1:B:236:PRO:HA	1:B:247:TRP:CD1	2.49	0.48
1:D:501:ILE:HG23	1:D:505:ARG:HG3	1.95	0.48
1:B:411:ASP:O	1:B:415:LYS:HE2	2.14	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:C:191:PRO:HA	1:C:350:PHE:HA	1.96	0.48
1:B:193:PRO:O	1:B:197:VAL:HG23	2.14	0.48
1:A:295:VAL:HG13	1:A:345:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:GLY:HA3	1:C:624:ARG:O	2.14	0.47
1:A:248:HIS:HA	1:A:271:CYS: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:C:147:ALA:HB2	1:C:452:TYR:CD1	2.43	0.47
1:A:550:ILE:O	1:A:553:VAL:HG12	2.14	0.47
1:D:175:PHE:HB3	1:D:258:ARG:HE	1.79	0.47
1:B:224:HIS:HE1	1:B:268:THR:HG23	1.77	0.47
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.79	0.47
1:D:438:GLN:HB3	1:D:439:PRO:HD2	1.97	0.47
1:C:106:ALA:HA	1:C:643:PHE:HE2	1.79	0.47
1:D:325:PHE:HB3	1:D:340:THR:O	2.14	0.47
1:D:706:GLN:O	1:D:710:GLN:HG3	2.15	0.47
1:A:377:ARG:HA	1:A:385:ARG:O	2.14	0.47
1:A:234:LEU:HD23	1:A:249:THR:HG23	1.96	0.47
1:C:332:THR:C	1:C:334:ALA:H	2.17	0.47
1:C:629:ALA:C	1:C:630:ILE:HD12	2.35	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
1:D:658:GLN:C	1:D:659:LEU:HD12	2.36	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:D:528:TRP:O	1:D:532:GLN:HG2	2.16	0.46
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.96	0.46
1:C:347:THR:HB	1:C:348:PRO:HD2	1.98	0.46
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.31	0.46
1:C:599:ARG:HD3	1:C:617:LEU:O	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:A:652:GLU:HA	1:A:652:GLU:OE1	2.16	0.46
1:D:377:ARG:HD2	1:D:377:ARG:C	2.36	0.46
1:D:114:TYR:HA	1:D:574:VAL:O	2.16	0.46
1:C:467:GLU:CD	1:C:470:ARG:HH22	2.18	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:A:119:PRO:HG3	1:A:561:ALA:HA	1.98	0.46
1:D:215:ARG:NH2	1:D:349:LYS:HD3	2.31	0.46
1:B:546:ASN:HB3	1:B:550:ILE:HD13	1.98	0.46
1:B:377:ARG:HA	1:B:385:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:366:MET:HE1	1:C:495:ILE:HG21	1.98	0.45
1:B:388:SER:OG	1:B:391:ILE:HG12	2.16	0.45
1:D:500:SER:OG	1:D:502:GLU:HG2	2.16	0.45
1:B:607:GLU:H	1:B:607:GLU:HG2	1.53	0.45
1:A:402:TYR:HA	1:A:403:PRO:HD3	1.86	0.45
1:C:325:PHE:O	1:C:339:PRO:HA	2.15	0.45
1:D:601:LEU:HD23	1:D:616:GLN:HB3	1.98	0.45
1:D:209:SER:HB3	1:D:230:THR:H	1.82	0.45
1:C:209:SER:HB2	1:C:224:HIS:CB	2.47	0.45
1:A:397:THR:HG22	1:A:398:ASN:N	2.32	0.45
1:D:250:THR:HG22	1:D:251:ASP:H	1.82	0.45
1:D:115:VAL:O	1:D:117:PRO:HD3	2.17	0.45
1:B:248:HIS:HB2	1:B:270:ASN:OD1	2.17	0.45
1:D:301:TYR:HA	1:D:307:SER:O	2.17	0.45
1:A:188:ASP:OD1	1:A:215:ARG:NH2	2.48	0.45
1:B:365:THR:O	1:B:366:MET:HE2	2.16	0.45
1:A:332:THR:C	1:A:334:ALA:H	2.20	0.45
1:B:286:GLU:HB2	1:B:296:TYR:HA	1.99	0.45
1:C:550:ILE:O	1:C:553:VAL:HG12	2.17	0.45
1:A:649:TYR:O	1:A:656:SER:HB3	2.16	0.45
1:D:252:LEU:N	1:D:252:LEU:HD12	2.31	0.45
1:B:597:TYR:CE1	1:B:601:LEU:HD11	2.52	0.45
1:B:113:PHE:O	1:B:575:PRO:HA	2.16	0.45
1:C:512:HIS:CE1	1:C:515:ARG:HH22	2.34	0.45
1:D:515:ARG:O	1:D:519:ASP:HB2	2.17	0.45
1:C:589:ILE:HG12	1:C:597:TYR:CE1	2.52	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: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:D:166:LYS:HE2	1:D:207:CYS:SG	2.57	0.44
1:C:421:MET:SD	1:C:453:GLN:HB2	2.57	0.44
1:D:165:TYR:HA	1:D:192:VAL:HG23	1.99	0.44
1:D:117:PRO:O	1:D:118:PRO:C	2.56	0.44
1:D:301:TYR:CD1	1:D:310:GLU:HB2	2.52	0.44
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.99	0.44
1:A:392:SER:HA	1:A:508:PHE:CE2	2.52	0.44
1:B:440:GLN:OE1	1:B:454:PRO:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:552:SER:HA	1:C:559:VAL:HG22	1.99	0.44
1:A:354:TRP:CE3	1:A:354:TRP:N	2.86	0.44
1:C:401:GLU:HG2	1:C:474:ARG:O	2.17	0.43
1:C:719:ILE:H	1:C:719:ILE:HD12	1.83	0.43
1:B:175:PHE:CG	1:B:258:ARG:HB3	2.53	0.43
1:B:162:THR:HA	1:B:274:GLU:O	2.18	0.43
1:B:263:HIS:NE2	1:B:265:TYR:CE2	2.86	0.43
1:C:318:ARG:O	1:C:346:THR:HG22	2.18	0.43
1:B:475:LYS:HA	1:B:476:PRO:HD3	1.87	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
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:D:155:ALA:HA	1:D:156:PRO:HD3	1.85	0.43
1:A:515:ARG:HD2	5:A:750:HOH:O	2.18	0.43
1:B:200:LYS:HE3	1:B:208:ARG:CZ	2.48	0.43
1:C:106:ALA:HA	1:C:643:PHE:CE2	2.53	0.43
1:B:332:THR:O	1:B:333:LYS:HB2	2.19	0.43
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.87	0.43
1:A:391:ILE:O	1:A:391:ILE:HG22	2.18	0.43
1:D:420:ALA:HA	1:D:423:ARG:CZ	2.48	0.43
1:A:347:THR:HB	1:A:348:PRO:HD2	2.00	0.43
1:C:402:TYR:CD1	1:C:403:PRO:HD2	2.53	0.43
1:A:718:ASP:OD1	1:A:718:ASP:C	2.57	0.43
1:B:302:GLY:O	1:B:308:HIS:HA	2.19	0.43
1:B:132:ARG:HH11	1:B:132:ARG:HB3	1.84	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: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:D:319:PHE:CZ	1:D:321:GLN:HB2	2.54	0.43
1:A:440:GLN:HE22	1:A:471:GLU:HB3	1.84	0.43
1:B:466:ARG:HH22	1:B:470:ARG:HB2	1.83	0.42
1:B:230:THR:CG2	1:B:231:ASP:N	2.82	0.42
1:C:360:ARG:HB2	1:C:361:PRO:HD3	2.01	0.42
1:B:341:THR:HB	1:B:356:TRP:HB3	2.01	0.42
1:C:436:VAL:HB	1:C:454:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PRO:HB2	1:A:406:ARG:HB2	2.01	0.42
1:B:718:ASP:HB3	1:B:721:THR:HG23	2.01	0.42
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.80	0.42
1:C:630:ILE:CG2	1:C:631:GLU:N	2.82	0.42
1:B:329:ASP:HB3	1:B:332:THR:OG1	2.20	0.42
1:C:129:GLN:HB3	1:C:130:PRO:HD2	2.01	0.42
1:C:634:THR:HB	1:C:637:HIS:HB2	2.01	0.42
1:B:585:ASN:OD1	1:B:585:ASN:N	2.50	0.42
1:D:190:ALA:HA	1:D:191:PRO:HD3	1.87	0.42
1:D:659:LEU:N	1:D:659:LEU:HD12	2.35	0.42
1:C:634:THR:O	1:C:653:TYR:HE1	2.03	0.42
1:C:519:ASP:O	1:C:523:ARG:HG3	2.19	0.42
1:D:147:ALA:HA	1:D:451:ALA:O	2.19	0.42
1:A:475:LYS:HA	1:A:476:PRO:HD3	1.90	0.42
1:A:298:SER:HB3	1:A:310:GLU:HB3	2.01	0.42
1:C:256:PRO:HD3	1:C:266:GLY:HA3	2.01	0.42
1:D:328:ARG:HH12	1:D:335:ARG:HB2	1.84	0.42
1:C:344:LEU:HA	1:C:352:VAL:O	2.19	0.42
1:D:255:ASN:HA	1:D:256:PRO:HD3	1.82	0.42
1:B:140:GLN:HB3	1:B:142:TYR:CE1	2.55	0.42
1:D:439:PRO:HD3	1:D:453:GLN:OE1	2.19	0.42
1:D:201:ILE:O	1:D:205:GLY:HA2	2.19	0.42
1:C:396:THR:O	1:C:444:ALA:HA	2.19	0.42
1:B:366:MET:CE	1:B:495:ILE:HB	2.50	0.42
1:D:442:TYR:O	1:D:449:LEU:HD12	2.20	0.42
1:D:171:SER:O	1:D:265:TYR:HB2	2.20	0.42
1:C:325:PHE:HB3	1:C:340:THR:O	2.19	0.42
1:A:596:CYS:HB3	1:A:653:TYR:CE2	2.55	0.42
1:D:522:GLY:O	1:D:526:ILE:HG13	2.20	0.42
1:A:248:HIS:HE1	1:A:251:ASP:OD2	2.02	0.42
1:A:240:ALA:HB3	1:A:243:THR:HG21	2.01	0.42
1:D:282:TYR:CG	1:D:283:PRO:HA	2.55	0.42
1:B:621:ASN:OD1	1:B:643:PHE:HA	2.20	0.42
1:A:545:LEU:O	1:A:547:PRO:HD3	2.20	0.42
1:C:513:ILE:O	1:C:514:GLN:C	2.58	0.42
1:D:402:TYR:HA	1:D:403:PRO:HD3	1.87	0.41
1:B:621:ASN:ND2	1:B:644:GLY:H	2.18	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:D:201:ILE:HG12	1:D:206:VAL:O	2.20	0.41
1:C:125:VAL:O	1:C:567:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:VAL:HG13	1:C:518:ASN:H	1.83	0.41
1:C:163:MET:O	1:C:273:VAL:HG13	2.19	0.41
1:D:298:SER:C	1:D:300:PHE:H	2.23	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:D:209:SER:OG	1:D:224:HIS:HB3	2.21	0.41
1:A:512:HIS:CE1	1:A:515:ARG:HH12	2.39	0.41
1:B:147:ALA:HA	1:B:451:ALA:O	2.20	0.41
1:D:174:TRP:HZ3	1:D:179:TYR:HH	1.67	0.41
1:C:555:VAL:HG13	1:C:557:ARG:HG2	2.02	0.41
1:D:502:GLU:HG3	1:D:503:PHE:H	1.85	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:C:377:ARG:HB3	1:C:377:ARG:HH11	1.86	0.41
1:B:244:SER:O	3:B:4000:MRY:HAE	2.20	0.41
1:C:401:GLU:OE1	1:C:440:GLN:HB2	2.21	0.41
1:B:194:PHE:CD2	1:B:320:LYS:HD2	2.55	0.41
1:B:190:ALA:HA	1:B:191:PRO:HD3	1.83	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:587:MET:HG3	1:A:650:PHE:CE2	2.55	0.41
1:D:298:SER:HA	1:D:299:PRO:HD3	1.91	0.41
1:A:561:ALA:HB2	1:A:570:VAL:HG12	2.03	0.41
1:D:191:PRO:HA	1:D:350:PHE:HA	2.02	0.41
1:D:120:THR:C	1:D:122:ALA:H	2.24	0.41
1:A:106:ALA:HA	1:A:643:PHE:CE2	2.56	0.41
1:B:163:MET:O	1:B:273:VAL:HA	2.21	0.41
1:D:236:PRO:HA	1:D:247:TRP:CD1	2.55	0.40
1:A:285:ASP:HB2	1:A:311:HIS:HB3	2.03	0.40
1:C:155:ALA:HA	1:C:156:PRO:HD3	1.92	0.40
1:B:397:THR:HG22	1:B:444:ALA:HA	2.01	0.40
1:B:588:ARG:HA	1:B:596:CYS:SG	2.60	0.40
1:C:259:VAL:HG23	1:C:260:GLU:CD	2.42	0.40
1:C:104:ILE:O	1:C:582:ILE:HG23	2.21	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:D:197:VAL:O	1:D:201:ILE:HB	2.22	0.40
1:C:192:VAL:HG11	1:C:201:ILE:CD1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:386:PHE:HB2	1:D:395:PHE:HB2	2.04	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:B:174:TRP:CD1	1:B:174:TRP:C	2.93	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%)	26 70
1	B	591/703 (84%)	543 (92%)	47 (8%)	1 (0%)	52 88
1	C	597/703 (85%)	543 (91%)	52 (9%)	2 (0%)	46 84
1	D	599/703 (85%)	535 (89%)	61 (10%)	3 (0%)	34 76
All	All	2386/2812 (85%)	2165 (91%)	211 (9%)	10 (0%)	39 80

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
1	A	517	VAL
1	D	134	PRO

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Mol	Chain	Res	Type
1	A	324	GLY
1	C	413	ILE

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	512/593 (86%)	495 (97%)	17 (3%)	45 82
1	B	507/593 (86%)	482 (95%)	25 (5%)	31 71
1	C	494/593 (83%)	474 (96%)	20 (4%)	38 77
1	D	511/593 (86%)	482 (94%)	29 (6%)	25 64
All	All	2024/2372 (85%)	1933 (96%)	91 (4%)	34 74

All (91) 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	263	HIS
1	A	309	THR
1	A	384	PHE
1	A	387	SER
1	A	404	LEU
1	A	463	LEU
1	A	492	VAL
1	A	502	GLU
1	A	584	GLN
1	A	608	ASP
1	B	124	VAL
1	B	177	HIS

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Mol	Chain	Res	Type
1	B	181	GLN
1	B	217	ASN
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	384	PHE
1	B	389	ASP
1	B	401	GLU
1	B	440	GLN
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	691	ARG
1	B	721	THR
1	C	108	ASN
1	C	120	THR
1	C	189	ARG
1	C	241	THR
1	C	258	ARG
1	C	271	CYS
1	C	346	THR
1	C	377	ARG
1	C	392	SER
1	C	464	TYR
1	C	512	HIS
1	C	529	CYS
1	C	530	GLU
1	C	546	ASN
1	C	567	VAL
1	C	584	GLN
1	C	660	SER
1	C	711	LEU
1	C	719	ILE

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Mol	Chain	Res	Type
1	C	722	VAL
1	D	140	GLN
1	D	167	ASP
1	D	179	TYR
1	D	189	ARG
1	D	228	HIS
1	D	241	THR
1	D	248	HIS
1	D	252	LEU
1	D	258	ARG
1	D	311	HIS
1	D	313	SER
1	D	323	ASP
1	D	389	ASP
1	D	401	GLU
1	D	412	CYS
1	D	428	ARG
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	585	ASN
1	D	608	ASP
1	D	609	GLN
1	D	634	THR
1	D	635	VAL
1	D	648	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	112	ASN
1	A	532	GLN
1	B	468	HIS
1	C	453	GLN
1	C	709	ASN
1	C	710	GLN
1	D	140	GLN

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Mol	Chain	Res	Type
1	D	181	GLN
1	D	609	GLN
1	D	709	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 carbohydrates in this entry.

5.6 Ligand geometry

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	0.48	0	15,19,21	1.18	2 (13%)
2	NAG	A	1398	1	14,14,15	0.55	0	15,19,21	0.67	0
2	NAG	A	1674	1	14,14,15	0.46	0	15,19,21	0.92	1 (6%)
3	MRY	A	4000	-	7,7,7	0.55	0	6,8,8	1.09	0
2	NAG	B	1430	1	14,14,15	0.61	0	15,19,21	0.92	1 (6%)
3	MRY	B	4000	-	7,7,7	0.58	0	6,8,8	0.95	0
2	NAG	C	1141	1	14,14,15	0.50	0	15,19,21	1.00	2 (13%)
2	NAG	C	1398	1	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
2	NAG	C	1674	1	14,14,15	0.48	0	15,19,21	0.82	0
2	NAG	D	1141	1	14,14,15	0.49	0	15,19,21	0.81	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
2	NAG	A	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1398	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	MRY	A	4000	-	-	0/8/8/8	0/0/0/0
2	NAG	B	1430	1	-	0/6/23/26	0/1/1/1
3	MRY	B	4000	-	-	0/8/8/8	0/0/0/0
2	NAG	C	1141	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1398	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1141	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1674	NAG	C2-N2-C7	-2.18	120.24	123.04
2	C	1141	NAG	C2-N2-C7	-2.17	120.25	123.04
2	A	1141	NAG	C2-N2-C7	-2.07	120.38	123.04
2	C	1398	NAG	C1-O5-C5	2.19	115.03	112.25
2	C	1141	NAG	C1-O5-C5	2.47	115.38	112.25
2	B	1430	NAG	C1-O5-C5	2.48	115.39	112.25
2	A	1141	NAG	C1-O5-C5	3.17	116.27	112.25

There are no chirality outliers.

There are no torsion outliers.

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
2	A	1398	NAG	1	0
3	B	4000	MRY	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	605/703 (86%)	-0.41	6 (0%)	84	60	5, 46, 115, 474	0
1	B	596/703 (84%)	-0.38	5 (0%)	87	67	9, 53, 129, 232	0
1	C	603/703 (85%)	-0.29	5 (0%)	87	67	19, 72, 139, 454	0
1	D	605/703 (86%)	-0.38	6 (0%)	84	60	17, 62, 124, 292	0
All	All	2409/2812 (85%)	-0.36	22 (0%)	85	64	5, 59, 129, 474	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	595	ALA	8.1
1	B	591	SER	5.3
1	C	577	ALA	5.0
1	D	336	ALA	4.4
1	A	650	PHE	4.3
1	C	597	TYR	3.9
1	A	577	ALA	3.8
1	A	595	ALA	3.6
1	D	653	TYR	3.4
1	B	653	TYR	3.2
1	C	465	VAL	2.8
1	B	623	LEU	2.7
1	B	464	TYR	2.7
1	B	604	PHE	2.7
1	D	207	CYS	2.6
1	A	111	ALA	2.5
1	D	591	SER	2.5
1	D	632	PRO	2.2
1	A	580	ASN	2.2
1	C	303	TYR	2.2
1	A	492	VAL	2.2
1	D	110	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MRY	A	4000	8/8	0.91	0.26	5.72	54,54,54,54	0
3	MRY	B	4000	8/8	0.94	0.14	-0.28	47,47,47,47	0
2	NAG	A	1398	14/15	0.96	0.09	-3.42	52,58,58,58	0
2	NAG	C	1141	14/15	0.89	0.13	-	113,113,113,113	0
2	NAG	B	1430	14/15	0.93	0.13	-	85,85,85,85	0
2	NAG	C	1674	14/15	0.93	0.10	-	87,87,87,87	0
2	NAG	D	1141	14/15	0.85	0.22	-	116,116,116,116	0
2	NAG	A	1141	14/15	0.93	0.10	-	81,81,81,81	0
2	NAG	C	1398	14/15	0.92	0.11	-	94,94,94,94	0
2	NAG	A	1674	14/15	0.95	0.10	-	73,73,73,73	0
4	NA	A	751	1/1	0.90	0.27	-	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.