



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2023 – 01:33 AM EDT

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

<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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

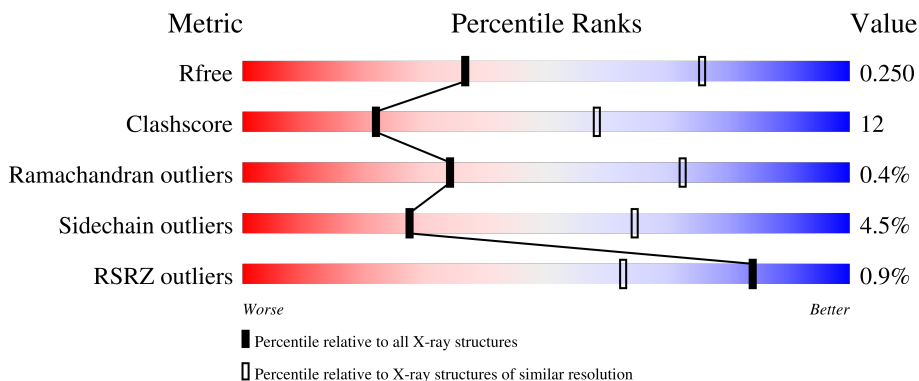
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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
			Total	C	N	O	S			
1	A	605	4814	3040	845	907	22	0	0	0
1	B	596	4762	3012	837	891	22	0	1	0
1	C	603	4727	2985	814	907	21	0	0	0
1	D	605	4813	3036	841	914	22	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

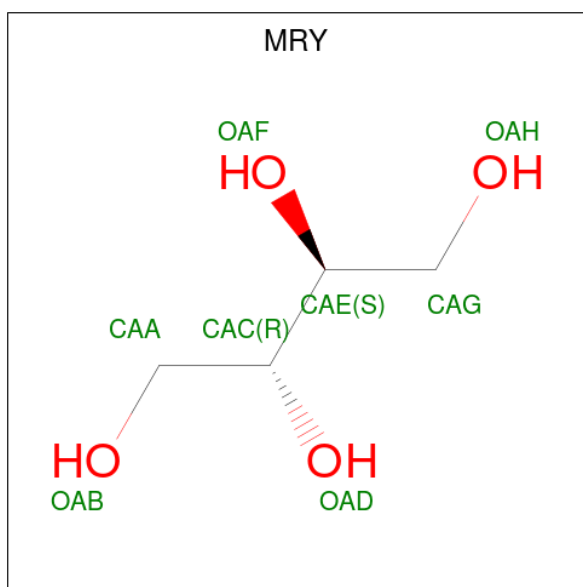
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	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 (three-letter code: 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 (three-letter code: MRY) (formula: $C_4H_{10}O_4$).



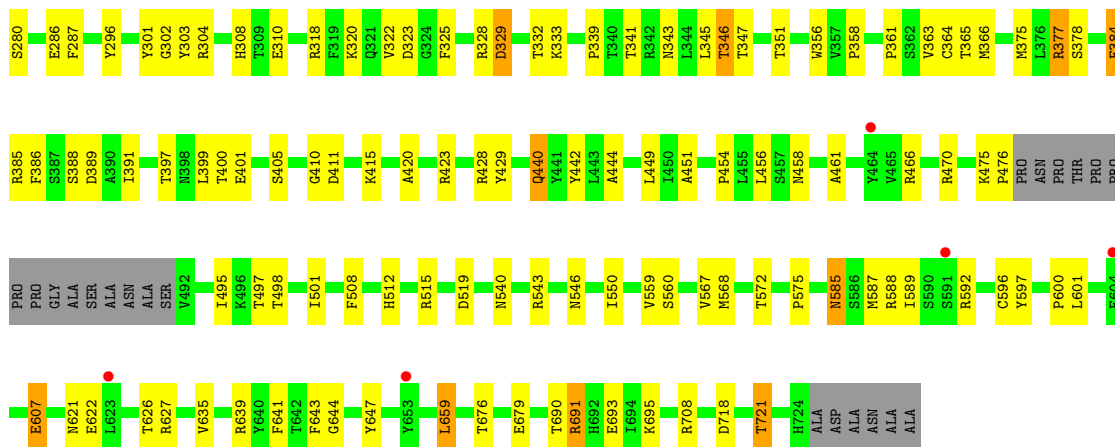
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 4 4	0	0
3	B	1	Total C O 8 4 4	0	0

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

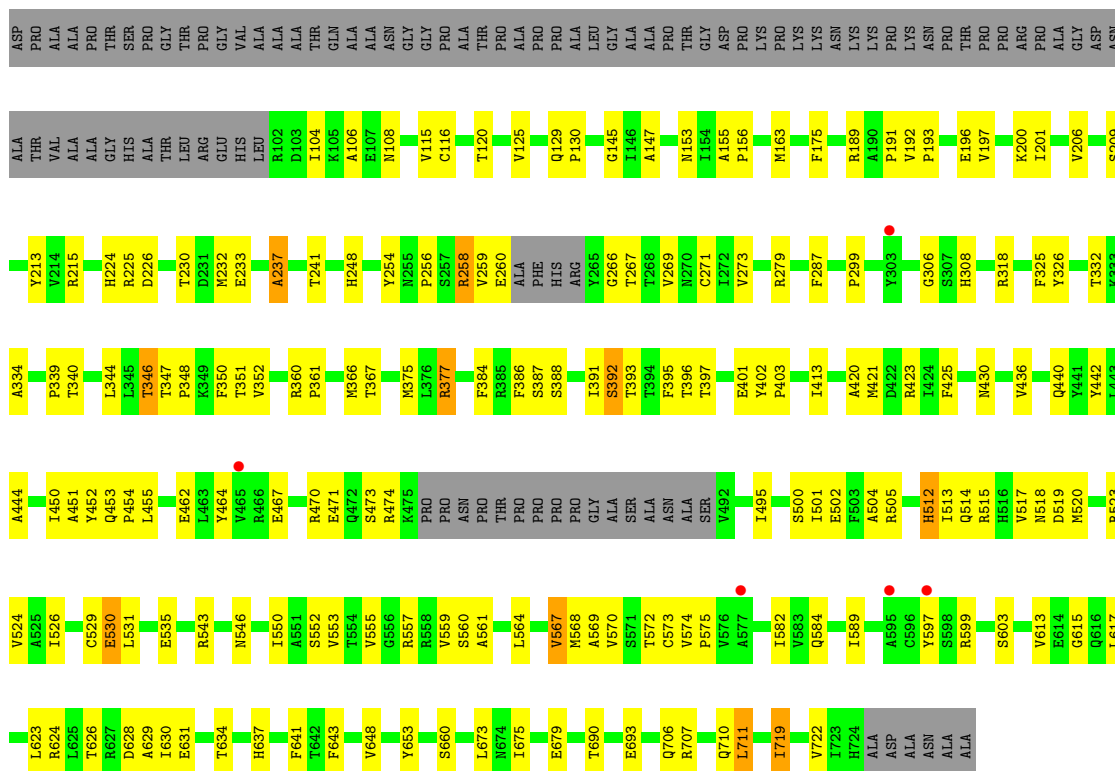
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

- Molecule 5 is water.

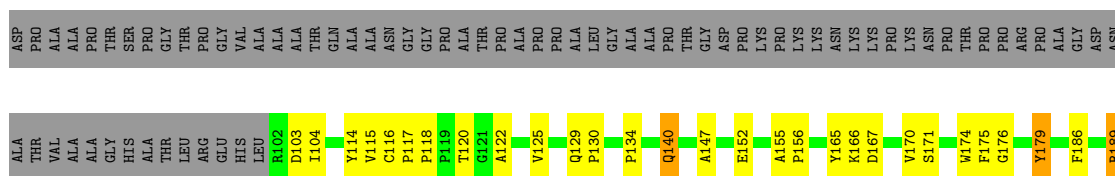
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	17	Total O 17 17	0	0
5	C	12	Total O 12 12	0	0
5	D	15	Total O 15 15	0	0

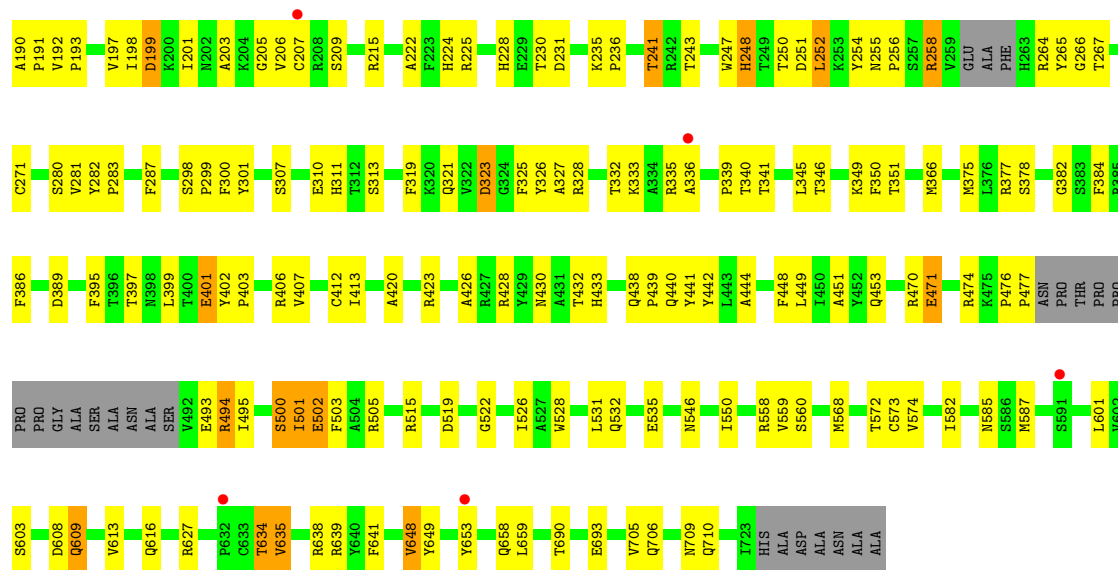


• Molecule 1: Envelope glycoprotein B



• Molecule 1: Envelope glycoprotein B





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
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.81Å)	Xtrriage
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	5715 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtrriage
Anisotropy	0.016	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l 0.460 for h,-h-k,-l 0.039 for -k,-h,-l	Xtrriage
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

Xtrriage'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: NAG, NA, 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 [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	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:C	1:B:265:TYR:HD2	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:B:265:TYR:C	1:B:265:TYR:CD2	2.67	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:679:GLU:CD	1:C:679:GLU:H	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: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
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: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: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
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:D:129:GLN:HB3	1:D:130:PRO:HD2	1.88	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

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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: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: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: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
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: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: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: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: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: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: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:C:462:GLU:CD	1:C:462:GLU:H	2.14	0.50
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
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: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: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: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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:377:ARG:C	1:D:377:ARG:HD2	2.36	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:C:467:GLU:CD	1:C:470:ARG:HH22	2.18	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

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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:C:366:MET:HE1	1:C:495:ILE:HG21	1.98	0.45
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: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: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:A:332:THR:C	1:A:334:ALA:H	2.20	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: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: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: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:117:PRO:O	1:D:118:PRO:C	2.56	0.44
1:D:165:TYR:HA	1:D:192:VAL:HG23	1.99	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: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: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: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
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: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:A:718:ASP:C	1:A:718:ASP:OD1	2.57	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: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:D:319:PHE:CZ	1:D:321:GLN:HB2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:475:LYS:HA	1:A:476:PRO:HD3	1.90	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: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: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:C:513:ILE:O	1:C:514:GLN:C	2.58	0.42
1:D:282:TYR:CG	1:D:283:PRO:HA	2.55	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

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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:D:201:ILE:HG12	1:D:206:VAL:O	2.20	0.41
1:D:114:TYR:HB3	1:D:573:CYS:HB3	2.03	0.41
1:D:298:SER:C	1:D:300:PHE:H	2.23	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
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:C:555:VAL:HG13	1:C:557:ARG:HG2	2.02	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: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:587:MET:HG3	1:A:650:PHE:CE2	2.55	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:D:120:THR:C	1:D:122:ALA:H	2.24	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: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: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:C:259:VAL:HG23	1:C:260:GLU:CD	2.42	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
1:D:197:VAL:O	1:D:201:ILE:HB	2.22	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:B:156:PRO:O	1:B:158:LYS:HD2	2.22	0.40
1:B:174:TRP:CD1	1:B:174:TRP:C	2.93	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%)	22	60
1	B	591/703 (84%)	543 (92%)	47 (8%)	1 (0%)	47	82
1	C	597/703 (85%)	543 (91%)	52 (9%)	2 (0%)	41	76
1	D	599/703 (85%)	535 (89%)	61 (10%)	3 (0%)	29	68
All	All	2386/2812 (85%)	2165 (91%)	211 (9%)	10 (0%)	34	72

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%)	38 73
1	B	507/593 (86%)	482 (95%)	25 (5%)	25 61
1	C	494/593 (83%)	474 (96%)	20 (4%)	31 68
1	D	511/593 (86%)	482 (94%)	29 (6%)	20 56
All	All	2024/2372 (85%)	1933 (96%)	91 (4%)	27 64

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

Sometimes 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 [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 monosaccharides 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	$\# Z > 2$
3	MRY	B	4000	-	7,7,7	0.61	0	8,8,8	0.87	0
2	NAG	C	1141	1	14,14,15	0.53	0	17,19,21	0.91	1 (5%)
2	NAG	D	1141	1	14,14,15	0.52	0	17,19,21	0.76	0
2	NAG	A	1141	1	14,14,15	0.50	0	17,19,21	1.17	1 (5%)
3	MRY	A	4000	-	7,7,7	0.57	0	8,8,8	0.94	0
2	NAG	A	1398	1	14,14,15	0.58	0	17,19,21	0.76	0
2	NAG	A	1674	1	14,14,15	0.48	0	17,19,21	0.87	0
2	NAG	B	1430	1	14,14,15	0.63	0	17,19,21	0.96	1 (5%)
2	NAG	C	1398	1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
2	NAG	C	1674	1	14,14,15	0.50	0	17,19,21	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRY	B	4000	-	-	1/8/8/8	-
2	NAG	C	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	A	1141	1	-	0/6/23/26	0/1/1/1
3	MRY	A	4000	-	-	0/8/8/8	-
2	NAG	A	1398	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1430	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1398	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1674	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	3.01	116.27	112.19
2	B	1430	NAG	C1-O5-C5	2.36	115.39	112.19
2	C	1141	NAG	C1-O5-C5	2.35	115.38	112.19
2	C	1398	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1398	NAG	C4-C5-C6-O6
2	A	1398	NAG	O5-C5-C6-O6
2	B	1430	NAG	C1-C2-N2-C7
2	C	1398	NAG	O5-C5-C6-O6
2	D	1141	NAG	O5-C5-C6-O6
3	B	4000	MRY	OAD-CAC-CAE-OAF

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4000	MRY	3	0
2	A	1141	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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

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	605/703 (86%)	-0.42	6 (0%) 82 59	5, 46, 115, 474	0
1	B	596/703 (84%)	-0.40	5 (0%) 86 65	9, 53, 129, 232	0
1	C	603/703 (85%)	-0.31	5 (0%) 86 65	19, 72, 139, 454	0
1	D	605/703 (86%)	-0.39	5 (0%) 86 65	17, 62, 124, 292	0
All	All	2409/2812 (85%)	-0.38	21 (0%) 84 63	5, 59, 129, 474	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	595	ALA	7.9
1	B	591	SER	5.2
1	C	577	ALA	4.9
1	D	336	ALA	4.3
1	A	650	PHE	4.2
1	C	597	TYR	3.7
1	A	577	ALA	3.7
1	A	595	ALA	3.5
1	D	653	TYR	3.2
1	B	653	TYR	3.1
1	C	465	VAL	2.7
1	B	623	LEU	2.6
1	B	464	TYR	2.6
1	B	604	PHE	2.6
1	D	207	CYS	2.5
1	A	111	ALA	2.5
1	D	591	SER	2.4
1	D	632	PRO	2.2
1	A	580	ASN	2.1
1	A	492	VAL	2.1
1	C	303	TYR	2.1

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 monosaccharides 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(\AA^2)	Q<0.9
2	NAG	D	1141	14/15	0.85	0.22	116,116,116,116	0
2	NAG	C	1141	14/15	0.89	0.13	113,113,113,113	0
4	NA	A	751	1/1	0.90	0.27	63,63,63,63	0
3	MRY	A	4000	8/8	0.91	0.26	54,54,54,54	0
2	NAG	C	1398	14/15	0.92	0.11	94,94,94,94	0
2	NAG	A	1141	14/15	0.93	0.10	81,81,81,81	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
3	MRY	B	4000	8/8	0.94	0.14	47,47,47,47	0
2	NAG	A	1674	14/15	0.95	0.10	73,73,73,73	0
2	NAG	A	1398	14/15	0.96	0.09	52,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.