



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:35 PM UTC

PDB ID : 3D0H / pdb_00003d0h
Title : Crystal structure of spike protein receptor-binding domain from the 2002-2003 SARS coronavirus civet strain complexed with human-civet chimeric receptor ACE2
Authors : Li, F.
Deposited on : 2008-05-01
Resolution : 3.10 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

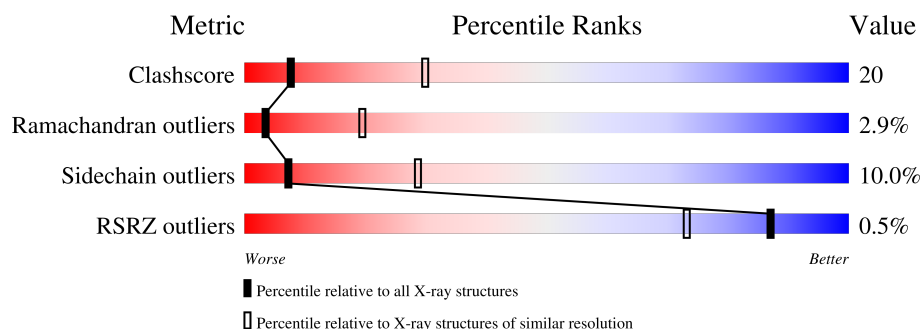
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	597	56%38%6%
1	B	597	56%37%7%
2	E	179	60%26%8% . .
2	F	179	53%36%7% . .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12643 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4864	3110	803	922	29			
1	B	597	Total	C	N	O	S	0	0	0
			4864	3110	803	922	29			

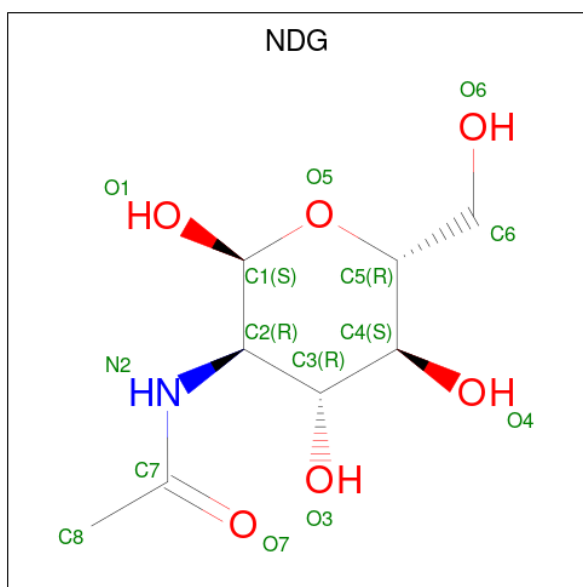
- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	173	Total	C	N	O	S	0	0	0
			1397	907	227	257	6			
2	F	173	Total	C	N	O	S	0	0	0
			1397	907	227	257	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	479	LYS	ASN	conflict	UNP P59594
E	487	SER	THR	conflict	UNP P59594
F	479	LYS	ASN	conflict	UNP P59594
F	487	SER	THR	conflict	UNP P59594

- Molecule 3 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	F	1	Total	C	N	O	0	0
			15	8	1	6		

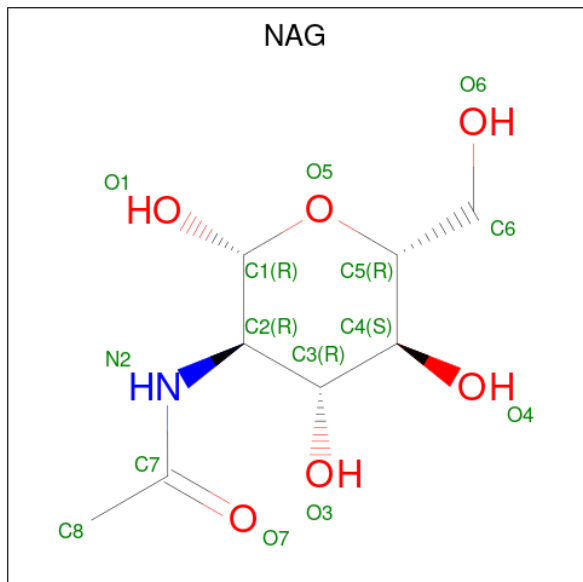
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	N	O	0	0
			15	8	1	6		

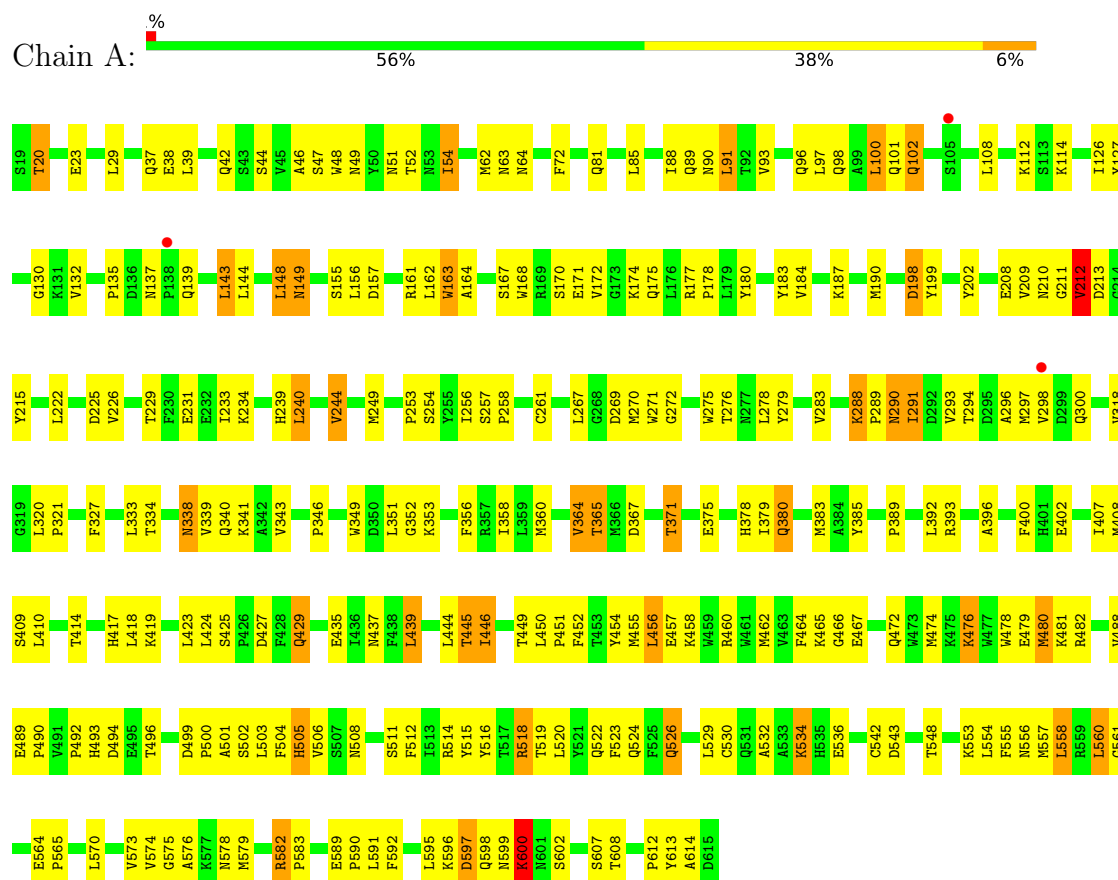
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	21	Total	O	0	0
			21	21		
7	F	6	Total	O	0	0
			6	6		

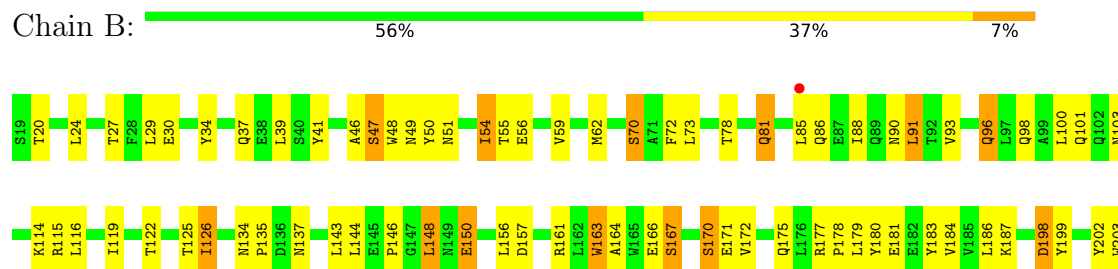
3 Residue-property plots

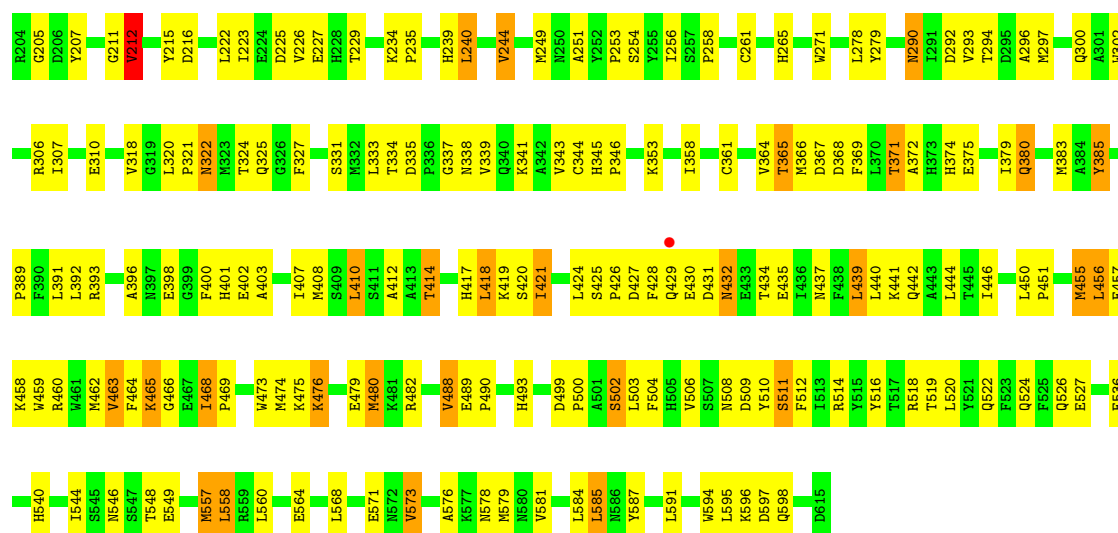
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Angiotensin-converting enzyme 2

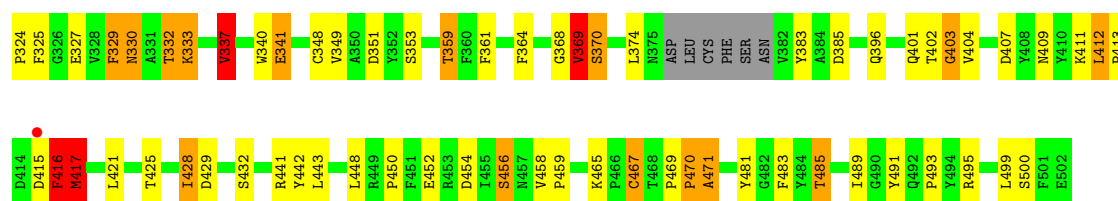


• Molecule 1: Angiotensin-converting enzyme 2

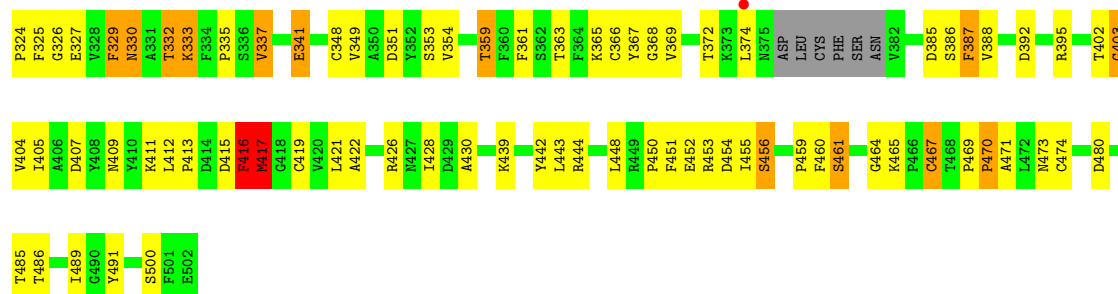




• Molecule 2: Spike glycoprotein



• Molecule 2: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.35Å 119.84Å 109.42Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	37.50 – 3.10 37.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.3 (37.50-3.10) 90.2 (37.50-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.302 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12643	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, CL, NAG, ZN

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	0.60	0/5000	0.94	6/6796 (0.1%)
1	B	0.65	0/5000	0.96	7/6796 (0.1%)
2	E	0.63	0/1442	0.93	3/1961 (0.2%)
2	F	0.62	0/1442	0.93	5/1961 (0.3%)
All	All	0.63	0/12884	0.94	21/17514 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	403	GLY	N-CA-C	8.16	123.92	110.55
1	A	291	ILE	N-CA-C	-8.00	104.77	112.29
2	E	417	MET	N-CA-C	7.69	118.73	107.88
1	A	290	ASN	N-CA-C	7.58	122.11	108.69
1	A	578	ASN	N-CA-C	7.55	119.15	108.74
2	E	403	GLY	N-CA-C	7.46	121.32	110.80
1	A	446	ILE	CB-CA-C	-7.31	102.52	111.88
2	F	417	MET	N-CA-C	7.22	119.50	108.52
2	F	461	SER	CA-C-N	6.32	126.01	119.82
2	F	461	SER	C-N-CA	6.32	126.01	119.82
1	B	465	LYS	N-CA-C	-6.16	105.86	113.19
1	B	468	ILE	CA-C-N	5.70	125.89	120.31
1	B	468	ILE	C-N-CA	5.70	125.89	120.31
2	F	359	THR	N-CA-C	-5.53	106.58	113.38
1	A	423	LEU	N-CA-C	-5.46	106.75	113.41
1	B	414	THR	CA-C-N	5.44	125.52	119.32
1	B	414	THR	C-N-CA	5.44	125.52	119.32
1	B	421	ILE	CB-CA-C	-5.30	104.91	111.70
1	B	256	ILE	N-CA-C	5.23	116.91	108.85
2	E	337	VAL	CB-CA-C	-5.14	105.31	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	N-CA-C	5.11	119.47	112.88

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	4864	0	4638	189	0
1	B	4864	0	4638	198	0
2	E	1397	0	1330	47	0
2	F	1397	0	1330	64	0
3	A	15	0	12	1	0
3	B	45	0	36	3	0
3	F	15	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	E	15	0	15	0	0
7	B	21	0	0	2	0
7	F	6	0	0	2	0
All	All	12643	0	12011	494	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 20.

All (494) 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:B:460:ARG:HH21	1:B:506:VAL:HA	1.29	0.94
1:B:460:ARG:NH2	1:B:506:VAL:HA	1.85	0.91
1:A:472:GLN:O	1:A:476:LYS:HB2	1.76	0.85
1:A:51:ASN:HD22	1:A:343:VAL:HG21	1.42	0.84
1:A:520:LEU:HD23	1:A:579:MET:HG2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TRP:HA	1:A:481:LYS:HB2	1.62	0.79
2:E:442:TYR:CD1	2:E:443:LEU:HG	2.17	0.79
1:A:574:VAL:HG23	1:A:576:ALA:H	1.49	0.77
1:B:175:GLN:O	1:B:178:PRO:HD2	1.85	0.76
1:B:459:TRP:O	1:B:463:VAL:HG23	1.85	0.76
2:E:454:ASP:OD2	2:E:456:SER:HB3	1.85	0.76
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.65	0.76
1:B:179:LEU:HD12	1:B:179:LEU:H	1.52	0.74
1:B:293:VAL:HG22	1:B:366:MET:HG3	1.67	0.74
2:F:361:PHE:CE2	2:F:421:LEU:HD23	2.22	0.74
1:A:600:LYS:HE3	1:A:600:LYS:HA	1.70	0.74
1:B:419:LYS:HD3	1:B:428:PHE:HB3	1.67	0.74
2:E:404:VAL:H	2:E:407:ASP:HB2	1.52	0.73
1:A:592:PHE:CE2	1:A:596:LYS:HD2	2.23	0.73
1:B:37:GLN:HE21	1:B:393:ARG:HH12	1.37	0.73
1:B:407:ILE:HD11	1:B:522:GLN:O	1.89	0.73
1:B:546:ASN:HD21	3:B:618:NDG:C1	2.01	0.73
1:A:225:ASP:O	1:A:229:THR:HG22	1.89	0.72
1:A:279:TYR:OH	1:A:437:ASN:HB3	1.90	0.72
1:B:306:ARG:O	1:B:310:GLU:HB2	1.89	0.71
1:B:557:MET:HE3	1:B:558:LEU:HA	1.71	0.71
1:B:51:ASN:HD22	1:B:343:VAL:HG21	1.55	0.71
1:B:297:MET:HE3	1:B:307:ILE:HD11	1.73	0.71
2:F:459:PRO:HB2	2:F:467:CYS:CB	2.20	0.71
1:A:407:ILE:HD11	1:A:522:GLN:O	1.91	0.70
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.57	0.70
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.74	0.70
2:F:459:PRO:HB2	2:F:467:CYS:HB3	1.74	0.70
1:A:534:LYS:HE2	1:B:430:GLU:O	1.92	0.69
1:B:450:LEU:HB2	1:B:451:PRO:HD3	1.73	0.69
1:B:549:GLU:CD	1:B:549:GLU:H	2.00	0.69
1:A:85:LEU:HD22	1:A:101:GLN:HE22	1.57	0.69
1:B:455:MET:HE2	1:B:455:MET:O	1.92	0.69
2:E:329:PHE:O	2:E:330:ASN:HB2	1.91	0.69
2:E:442:TYR:CE1	2:E:443:LEU:HG	2.27	0.69
2:F:416:PHE:CD1	2:F:416:PHE:N	2.61	0.69
1:A:598:GLN:OE1	1:A:598:GLN:HA	1.91	0.69
2:E:324:PRO:HD2	2:E:348:CYS:SG	2.34	0.68
1:A:505:HIS:CD2	1:A:505:HIS:H	2.11	0.68
2:E:416:PHE:CD1	2:E:416:PHE:N	2.61	0.68
1:A:597:ASP:O	1:A:600:LYS:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASN:O	1:B:93:VAL:HG22	1.95	0.67
1:B:504:PHE:O	1:B:508:ASN:HB2	1.94	0.67
2:F:454:ASP:OD2	2:F:456:SER:HB3	1.95	0.66
2:E:349:VAL:HG13	2:E:374:LEU:HB3	1.76	0.66
1:A:275:TRP:HB3	1:A:278:LEU:HD12	1.77	0.66
1:A:556:ASN:O	1:A:560:LEU:HD11	1.96	0.66
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.79	0.66
2:F:416:PHE:H	2:F:416:PHE:HD1	1.39	0.65
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.79	0.65
1:A:520:LEU:HD23	1:A:579:MET:CG	2.26	0.65
1:B:407:ILE:HB	1:B:408:MET:HE2	1.78	0.65
1:B:240:LEU:O	1:B:244:VAL:HG13	1.97	0.65
1:A:318:VAL:O	1:A:548:THR:HA	1.97	0.65
1:A:501:ALA:HA	1:A:506:VAL:CG1	2.27	0.65
2:F:417:MET:HA	2:F:417:MET:HE2	1.79	0.65
1:B:379:ILE:O	1:B:383:MET:HG3	1.96	0.65
1:B:389:PRO:HG2	1:B:392:LEU:HD22	1.79	0.64
2:F:442:TYR:CD1	2:F:443:LEU:HG	2.32	0.64
1:A:90:ASN:O	1:A:93:VAL:HG22	1.97	0.64
2:E:351:ASP:C	2:E:353:SER:H	2.06	0.64
1:A:519:THR:O	1:A:522:GLN:HG2	1.97	0.64
1:B:402:GLU:HB3	1:B:518:ARG:CD	2.28	0.64
2:E:332:THR:HG23	2:E:333:LYS:HE3	1.80	0.64
2:E:417:MET:HE2	2:E:417:MET:HA	1.80	0.64
2:E:425:THR:HG21	2:E:495:ARG:HG3	1.80	0.63
1:B:54:ILE:HG13	1:B:341:LYS:O	1.98	0.63
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.80	0.63
1:A:458:LYS:HG3	1:A:462:MET:HE2	1.81	0.63
2:F:372:THR:CG2	2:F:374:LEU:HD12	2.29	0.63
1:B:198:ASP:OD1	1:B:465:LYS:HG2	1.99	0.62
1:B:215:TYR:CE2	1:B:568:LEU:HD23	2.35	0.62
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.81	0.62
1:A:261:CYS:HB2	1:A:488:VAL:HG13	1.80	0.62
1:A:229:THR:HG23	1:A:516:TYR:OH	2.00	0.62
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.82	0.61
2:F:411:LYS:O	2:F:450:PRO:HA	2.00	0.61
1:B:293:VAL:CG2	1:B:366:MET:HG3	2.30	0.61
1:A:135:PRO:HD3	1:A:163:TRP:HE1	1.65	0.61
1:A:249:MET:HE1	1:A:258:PRO:CD	2.30	0.61
1:A:167:SER:O	1:A:171:GLU:HG2	2.01	0.61
2:F:404:VAL:H	2:F:407:ASP:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:MET:HE1	1:A:258:PRO:HG3	1.82	0.61
1:B:166:GLU:O	1:B:170:SER:HB2	2.01	0.60
1:A:46:ALA:HB1	1:A:62:MET:HA	1.83	0.60
1:A:37:GLN:NE2	1:A:393:ARG:HH12	2.00	0.60
1:A:47:SER:HA	1:A:62:MET:HG2	1.83	0.60
1:B:571:GLU:HA	1:B:576:ALA:H	1.67	0.60
2:E:383:TYR:O	2:E:499:LEU:HA	2.01	0.60
2:F:341:GLU:HA	2:F:341:GLU:OE1	1.99	0.60
1:A:90:ASN:OD1	3:A:616:NDG:O1	2.20	0.60
2:F:329:PHE:CD2	2:F:329:PHE:N	2.70	0.60
1:A:170:SER:O	1:A:174:LYS:HD2	2.02	0.60
1:A:240:LEU:O	1:A:244:VAL:HG13	2.02	0.60
1:A:85:LEU:HD13	1:A:98:GLN:HB2	1.83	0.60
1:A:429:GLN:H	1:A:429:GLN:NE2	1.99	0.60
1:B:251:ALA:O	1:B:253:PRO:HD3	2.02	0.59
1:B:265:HIS:ND1	1:B:490:PRO:HG3	2.18	0.59
2:E:383:TYR:HB2	2:E:500:SER:HB2	1.83	0.59
2:F:395:ARG:HG2	7:F:11:HOH:O	2.01	0.59
1:B:85:LEU:HA	1:B:88:ILE:HD12	1.84	0.59
1:B:37:GLN:NE2	1:B:393:ARG:HH12	1.98	0.59
1:B:229:THR:HG23	1:B:516:TYR:OH	2.02	0.59
1:B:366:MET:HE1	1:B:441:LYS:NZ	2.16	0.59
1:A:320:LEU:HD13	1:A:380:GLN:HG2	1.84	0.59
1:A:199:TYR:O	1:A:202:TYR:HB3	2.03	0.59
1:A:338:ASN:O	1:A:340:GLN:N	2.36	0.59
1:A:407:ILE:HB	1:A:408:MET:HE2	1.85	0.59
1:A:505:HIS:HE1	1:A:515:TYR:OH	1.86	0.59
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.85	0.59
1:A:180:TYR:O	1:A:184:VAL:HG23	2.03	0.58
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.67	0.58
2:E:411:LYS:O	2:E:450:PRO:HA	2.02	0.58
2:F:442:TYR:CE1	2:F:443:LEU:HG	2.38	0.58
1:B:464:PHE:C	1:B:466:GLY:H	2.11	0.58
1:A:462:MET:HE1	1:A:480:MET:HE1	1.86	0.57
1:B:324:THR:O	1:B:327:PHE:N	2.37	0.57
1:B:476:LYS:O	1:B:480:MET:HG2	2.04	0.57
2:F:324:PRO:HD2	2:F:348:CYS:SG	2.43	0.57
2:F:459:PRO:HB2	2:F:467:CYS:HB2	1.86	0.57
1:B:364:VAL:HG12	1:B:364:VAL:O	2.04	0.57
1:A:143:LEU:HD12	1:A:143:LEU:H	1.68	0.57
1:B:37:GLN:HE22	1:B:393:ARG:HH22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:469:PRO:HA	2:E:471:ALA:N	2.20	0.56
1:B:474:MET:HE1	1:B:499:ASP:H	1.69	0.56
1:A:553:LYS:O	1:A:573:VAL:HG12	2.05	0.56
2:F:329:PHE:O	2:F:330:ASN:HB2	2.04	0.56
2:F:372:THR:HG22	2:F:374:LEU:HD12	1.86	0.56
1:A:91:LEU:H	1:A:91:LEU:HD12	1.70	0.56
1:B:46:ALA:HB1	1:B:62:MET:HA	1.88	0.56
1:B:166:GLU:OE1	1:B:493:HIS:HE1	1.88	0.56
2:F:329:PHE:O	2:F:330:ASN:CB	2.53	0.56
2:F:439:LYS:HD3	2:F:480:ASP:OD1	2.05	0.56
1:B:499:ASP:N	1:B:500:PRO:HD2	2.20	0.56
1:A:157:ASP:O	1:A:161:ARG:HG3	2.05	0.56
1:B:183:TYR:OH	1:B:509:ASP:OD1	2.17	0.56
2:F:363:THR:HB	2:F:422:ALA:HB3	1.87	0.56
2:F:403:GLY:HA2	2:F:407:ASP:CG	2.31	0.56
1:B:455:MET:HE2	1:B:455:MET:C	2.31	0.55
2:E:404:VAL:N	2:E:407:ASP:HB2	2.20	0.55
2:F:404:VAL:N	2:F:407:ASP:HB2	2.21	0.55
1:B:85:LEU:HD13	1:B:98:GLN:HB2	1.88	0.55
1:B:226:VAL:O	1:B:229:THR:HG22	2.07	0.55
1:B:564:GLU:OE1	1:B:568:LEU:HD12	2.07	0.55
2:E:409:ASN:HD21	2:E:441:ARG:H	1.53	0.55
1:A:352:GLY:O	1:A:353:LYS:C	2.49	0.55
1:B:504:PHE:C	1:B:504:PHE:CD2	2.85	0.55
1:A:85:LEU:HD22	1:A:101:GLN:NE2	2.19	0.55
1:A:557:MET:HA	1:A:560:LEU:HD13	1.88	0.55
2:E:361:PHE:CE2	2:E:421:LEU:HD23	2.41	0.55
1:B:234:LYS:HB2	1:B:235:PRO:HD3	1.88	0.55
1:A:455:MET:HE1	1:A:481:LYS:HG2	1.88	0.54
1:B:48:TRP:HD1	1:B:49:ASN:HD22	1.55	0.54
1:A:450:LEU:HD21	1:A:519:THR:HG21	1.88	0.54
1:B:581:VAL:HG22	1:B:585:LEU:HD22	1.88	0.54
2:F:413:PRO:HG2	2:F:416:PHE:O	2.08	0.54
1:A:560:LEU:HD12	1:A:560:LEU:N	2.23	0.54
1:B:293:VAL:HA	7:B:917:HOH:O	2.08	0.54
1:B:227:GLU:OE2	1:B:458:LYS:HE2	2.08	0.54
2:E:329:PHE:O	2:E:330:ASN:CB	2.56	0.54
1:A:37:GLN:HE21	1:A:393:ARG:HH12	1.56	0.54
1:A:63:ASN:O	1:A:64:ASN:C	2.50	0.54
1:A:446:ILE:HG21	1:A:523:PHE:HE2	1.73	0.54
1:A:482:ARG:HD3	1:A:608:THR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:SER:HB3	1:A:514:ARG:HH21	1.73	0.53
1:B:524:GLN:HE22	1:B:579:MET:HA	1.73	0.53
1:B:261:CYS:HB2	1:B:488:VAL:HG22	1.91	0.53
1:B:322:ASN:ND2	3:B:617:NDG:O7	2.42	0.53
1:A:455:MET:CE	1:A:481:LYS:HG2	2.39	0.53
1:B:511:SER:O	1:B:514:ARG:NH1	2.41	0.53
2:F:335:PRO:HG3	2:F:341:GLU:HB2	1.90	0.53
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.90	0.53
1:B:578:ASN:CG	1:B:579:MET:H	2.17	0.53
1:B:482:ARG:HG2	1:B:488:VAL:CG1	2.39	0.53
2:E:325:PHE:C	2:E:327:GLU:H	2.15	0.53
1:A:135:PRO:CD	1:A:163:TRP:HE1	2.22	0.53
1:A:249:MET:HE1	1:A:258:PRO:HD3	1.91	0.52
2:E:413:PRO:HG2	2:E:416:PHE:O	2.07	0.52
1:B:47:SER:HA	1:B:62:MET:HG2	1.90	0.52
2:F:448:LEU:HB3	2:F:452:GLU:HB3	1.91	0.52
1:A:501:ALA:HA	1:A:506:VAL:HG12	1.90	0.52
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.91	0.52
1:B:157:ASP:O	1:B:161:ARG:HG3	2.10	0.52
1:B:464:PHE:C	1:B:466:GLY:N	2.66	0.52
1:B:183:TYR:O	1:B:187:LYS:HB2	2.09	0.52
1:A:249:MET:HE1	1:A:258:PRO:CG	2.39	0.52
2:F:469:PRO:HA	2:F:471:ALA:N	2.25	0.52
1:A:100:LEU:C	1:A:102:GLN:H	2.18	0.52
1:B:51:ASN:HD22	1:B:343:VAL:CG2	2.23	0.52
2:E:359:THR:C	2:E:361:PHE:H	2.18	0.52
1:B:91:LEU:HD12	1:B:91:LEU:H	1.75	0.52
1:B:211:GLY:O	1:B:212:VAL:HG13	2.09	0.52
1:A:346:PRO:HB3	1:A:360:MET:HG3	1.93	0.51
1:B:251:ALA:C	1:B:253:PRO:HD3	2.35	0.51
1:B:115:ARG:O	1:B:119:ILE:HG12	2.11	0.51
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.92	0.51
1:A:211:GLY:O	1:A:212:VAL:HG13	2.09	0.51
1:A:375:GLU:O	1:A:378:HIS:HB2	2.11	0.51
1:B:134:ASN:HB3	1:B:137:ASN:HB3	1.92	0.51
1:B:474:MET:CE	1:B:499:ASP:H	2.23	0.51
2:F:367:TYR:HB2	2:F:417:MET:HB3	1.92	0.51
1:A:174:LYS:NZ	1:A:496:THR:CG2	2.73	0.51
2:F:326:GLY:O	2:F:330:ASN:HB2	2.10	0.51
2:F:359:THR:C	2:F:361:PHE:H	2.18	0.51
1:A:85:LEU:HA	1:A:88:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:459:PRO:CB	2:F:467:CYS:HB3	2.39	0.51
1:A:582:ARG:HB3	1:A:583:PRO:HD3	1.92	0.51
2:E:469:PRO:HA	2:E:470:PRO:C	2.35	0.51
1:B:414:THR:O	1:B:418:LEU:HD22	2.11	0.51
1:B:407:ILE:CD1	1:B:522:GLN:O	2.59	0.51
1:A:276:THR:OG1	1:A:445:THR:HG23	2.12	0.50
1:B:407:ILE:HD11	1:B:522:GLN:HA	1.94	0.50
2:E:329:PHE:CD2	2:E:329:PHE:N	2.77	0.50
1:B:327:PHE:HE2	1:B:358:ILE:HG13	1.76	0.50
1:B:442:GLN:O	1:B:446:ILE:HG13	2.12	0.50
1:A:256:ILE:HG22	1:A:257:SER:N	2.26	0.50
1:B:346:PRO:HG3	7:B:908:HOH:O	2.10	0.50
1:A:132:VAL:HG12	1:A:171:GLU:HG3	1.91	0.50
1:A:222:LEU:O	1:A:226:VAL:HG23	2.12	0.50
1:B:578:ASN:CG	1:B:579:MET:N	2.70	0.50
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.77	0.50
1:B:526:GLN:HA	1:B:526:GLN:NE2	2.27	0.50
1:A:48:TRP:HD1	1:A:49:ASN:HD22	1.58	0.50
1:A:356:PHE:HB3	1:A:379:ILE:HD12	1.94	0.50
1:B:177:ARG:HB3	1:B:178:PRO:HD3	1.94	0.50
1:A:574:VAL:HG23	1:A:575:GLY:N	2.26	0.49
1:B:489:GLU:CD	1:B:489:GLU:H	2.19	0.49
2:E:415:ASP:O	2:E:416:PHE:C	2.54	0.49
1:B:429:GLN:CD	1:B:429:GLN:H	2.20	0.49
1:B:198:ASP:CG	1:B:465:LYS:HG2	2.37	0.49
1:B:223:ILE:O	1:B:227:GLU:HG3	2.12	0.49
1:A:570:LEU:O	1:A:574:VAL:HG22	2.12	0.49
1:A:414:THR:HG21	1:A:542:CYS:O	2.12	0.49
1:A:454:TYR:C	1:A:454:TYR:CD2	2.90	0.49
2:F:443:LEU:HD13	2:F:460:PHE:CD2	2.47	0.49
1:A:457:GLU:OE2	1:A:460:ARG:HD3	2.13	0.49
2:E:483:PHE:CD1	2:E:493:PRO:HB3	2.48	0.49
1:A:501:ALA:HA	1:A:506:VAL:HG11	1.93	0.49
1:B:335:ASP:C	1:B:337:GLY:H	2.20	0.49
2:E:442:TYR:HD1	2:E:443:LEU:HG	1.75	0.49
2:F:415:ASP:O	2:F:416:PHE:C	2.54	0.49
1:A:46:ALA:O	1:A:47:SER:C	2.56	0.49
1:A:452:PHE:CD1	1:A:452:PHE:C	2.90	0.49
1:A:511:SER:HB3	1:A:514:ARG:NH2	2.27	0.49
1:A:555:PHE:HA	1:A:558:LEU:HB2	1.93	0.49
1:B:177:ARG:O	1:B:181:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ASP:O	1:B:229:THR:HG22	2.13	0.49
1:B:440:LEU:HA	1:B:591:LEU:HD21	1.95	0.49
2:E:459:PRO:HB2	2:E:467:CYS:CB	2.43	0.49
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.48	0.49
1:B:249:MET:HE1	1:B:258:PRO:CD	2.43	0.49
1:A:239:HIS:CE1	1:A:596:LYS:HA	2.48	0.49
1:A:349:TRP:HB3	1:A:351:LEU:CD1	2.43	0.49
1:B:163:TRP:O	1:B:164:ALA:C	2.56	0.49
1:B:546:ASN:ND2	3:B:618:NDG:C1	2.73	0.49
1:A:294:THR:HG23	1:A:365:THR:HA	1.94	0.48
2:E:341:GLU:O	2:E:385:ASP:HA	2.13	0.48
2:F:341:GLU:OE1	2:F:341:GLU:CA	2.60	0.48
2:F:453:ARG:CZ	2:F:455:ILE:HD11	2.43	0.48
1:A:425:SER:C	1:A:427:ASP:H	2.21	0.48
1:B:167:SER:O	1:B:171:GLU:HG2	2.13	0.48
1:B:344:CYS:O	1:B:345:HIS:C	2.56	0.48
1:A:505:HIS:CE1	1:A:515:TYR:HE2	2.31	0.48
1:A:127:TYR:HE2	1:A:502:SER:O	1.96	0.48
1:A:132:VAL:HG22	1:A:148:LEU:HD21	1.95	0.48
1:A:396:ALA:HB3	1:A:400:PHE:CG	2.48	0.48
2:F:325:PHE:C	2:F:327:GLU:H	2.19	0.48
1:A:465:LYS:C	1:A:467:GLU:H	2.22	0.48
1:A:492:PRO:HD3	1:A:613:TYR:CD2	2.49	0.48
2:F:443:LEU:O	2:F:444:ARG:HB2	2.14	0.48
1:B:166:GLU:OE1	1:B:493:HIS:CE1	2.65	0.48
2:F:351:ASP:C	2:F:353:SER:H	2.22	0.48
2:F:489:ILE:C	2:F:491:TYR:H	2.22	0.48
1:B:50:TYR:CE1	1:B:54:ILE:HG23	2.48	0.48
1:B:294:THR:HG23	1:B:365:THR:HA	1.95	0.48
2:F:337:VAL:HG13	2:F:387:PHE:CD1	2.48	0.48
1:B:85:LEU:HD22	1:B:101:GLN:HE22	1.79	0.48
1:B:98:GLN:HA	1:B:101:GLN:HB2	1.94	0.48
1:A:135:PRO:HD3	1:A:163:TRP:NE1	2.28	0.47
1:A:155:SER:O	1:A:161:ARG:HD2	2.13	0.47
1:A:318:VAL:HA	1:A:548:THR:H	1.78	0.47
1:B:403:ALA:N	1:B:518:ARG:HG3	2.30	0.47
1:B:456:LEU:C	1:B:456:LEU:CD1	2.87	0.47
1:A:407:ILE:HD12	1:A:526:GLN:HB2	1.97	0.47
1:B:56:GLU:O	1:B:59:VAL:HG12	2.14	0.47
2:E:409:ASN:ND2	2:E:441:ARG:H	2.12	0.47
2:F:392:ASP:HA	7:F:11:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:O	1:B:223:ILE:C	2.58	0.47
1:A:379:ILE:O	1:A:383:MET:HG3	2.15	0.47
1:B:460:ARG:NH1	1:B:510:TYR:O	2.45	0.47
1:B:594:TRP:CH2	1:B:598:GLN:HG3	2.49	0.47
1:B:331:SER:HB2	1:B:333:LEU:HD21	1.96	0.47
1:B:450:LEU:CB	1:B:451:PRO:HD3	2.43	0.47
1:B:482:ARG:HG2	1:B:488:VAL:HG12	1.97	0.47
1:B:544:ILE:C	1:B:544:ILE:HD12	2.40	0.47
2:F:426:ARG:O	2:F:430:ALA:HB3	2.13	0.47
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.96	0.47
1:B:557:MET:HE2	1:B:558:LEU:HD12	1.97	0.47
1:A:297:MET:HE2	1:A:364:VAL:HG12	1.97	0.47
2:F:351:ASP:OD2	2:F:354:VAL:HG23	2.15	0.47
1:A:591:LEU:HG	1:A:595:LEU:HD23	1.96	0.46
1:B:212:VAL:HG23	1:B:216:ASP:OD1	2.15	0.46
1:B:396:ALA:HB3	1:B:400:PHE:CG	2.51	0.46
2:E:351:ASP:C	2:E:353:SER:N	2.73	0.46
1:A:261:CYS:CB	1:A:488:VAL:HG13	2.45	0.46
1:B:450:LEU:HD11	1:B:584:LEU:HD11	1.96	0.46
2:E:361:PHE:HE2	2:E:421:LEU:HB3	1.81	0.46
1:A:320:LEU:HB3	1:A:321:PRO:CD	2.44	0.46
1:B:540:HIS:HA	1:B:587:TYR:CE1	2.50	0.46
1:B:85:LEU:HD22	1:B:101:GLN:NE2	2.30	0.46
2:F:341:GLU:O	2:F:385:ASP:HA	2.16	0.46
1:B:199:TYR:O	1:B:202:TYR:HB3	2.15	0.46
1:B:358:ILE:HD13	1:B:375:GLU:HB3	1.98	0.46
2:E:432:SER:HA	2:E:485:THR:HG22	1.98	0.46
1:B:211:GLY:C	1:B:212:VAL:HG22	2.40	0.46
2:F:325:PHE:C	2:F:327:GLU:N	2.73	0.46
1:A:474:MET:CE	1:A:499:ASP:H	2.28	0.46
1:B:125:THR:O	1:B:126:ILE:C	2.58	0.46
1:B:229:THR:OG1	1:B:520:LEU:HD21	2.16	0.46
2:E:396:GLN:HA	2:E:401:GLN:HG3	1.97	0.46
2:E:458:VAL:O	2:E:459:PRO:C	2.59	0.46
1:A:446:ILE:HG21	1:A:523:PHE:CE2	2.51	0.46
2:F:329:PHE:H	2:F:329:PHE:HD2	1.59	0.46
1:B:432:ASN:OD1	1:B:432:ASN:N	2.48	0.45
1:B:595:LEU:O	1:B:596:LYS:C	2.60	0.45
2:F:461:SER:HB3	2:F:464:GLY:O	2.16	0.45
2:F:469:PRO:HA	2:F:470:PRO:C	2.41	0.45
1:A:505:HIS:CE1	1:A:515:TYR:CE2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:HD2	1:A:380:GLN:OE1	2.16	0.45
1:A:190:MET:HE1	1:A:202:TYR:CZ	2.51	0.45
1:A:208:GLU:OE1	1:A:210:ASN:ND2	2.48	0.45
1:A:407:ILE:HG23	1:A:526:GLN:NE2	2.32	0.45
1:B:366:MET:HE1	1:B:441:LYS:CE	2.47	0.45
1:A:209:VAL:HG21	1:A:565:PRO:HB3	1.98	0.45
1:B:597:ASP:O	1:B:598:GLN:C	2.59	0.45
1:A:435:GLU:O	1:A:439:LEU:HD22	2.17	0.45
1:B:143:LEU:O	1:B:144:LEU:C	2.59	0.45
1:B:514:ARG:O	1:B:518:ARG:CB	2.64	0.45
1:A:44:SER:HB3	1:A:351:LEU:HG	1.97	0.45
1:A:419:LYS:HG2	1:A:424:LEU:HB3	1.99	0.45
1:A:598:GLN:OE1	1:A:598:GLN:CA	2.61	0.45
1:B:179:LEU:H	1:B:179:LEU:CD1	2.26	0.45
1:B:297:MET:CE	1:B:307:ILE:HD11	2.45	0.45
2:F:337:VAL:CG1	2:F:387:PHE:CD1	3.00	0.45
1:B:474:MET:O	1:B:475:LYS:C	2.59	0.45
2:E:369:VAL:HB	2:E:370:SER:H	1.42	0.45
2:F:460:PHE:CD2	2:F:460:PHE:C	2.95	0.45
1:A:38:GLU:O	1:A:42:GLN:HG3	2.17	0.44
1:A:149:ASN:HD22	1:A:149:ASN:HA	1.65	0.44
1:B:239:HIS:O	1:B:240:LEU:C	2.60	0.44
1:B:78:THR:O	1:B:81:GLN:HB2	2.18	0.44
1:B:557:MET:HE3	1:B:558:LEU:CA	2.43	0.44
1:A:175:GLN:O	1:A:178:PRO:HD2	2.17	0.44
1:A:135:PRO:CD	1:A:163:TRP:NE1	2.80	0.44
1:A:174:LYS:HZ1	1:A:496:THR:CG2	2.30	0.44
1:A:379:ILE:CG2	1:A:383:MET:HE3	2.48	0.44
1:B:41:TYR:HH	2:F:486:THR:HG1	1.53	0.44
1:A:163:TRP:O	1:A:164:ALA:C	2.61	0.44
1:A:489:GLU:O	1:A:489:GLU:HG2	2.18	0.44
1:A:183:TYR:O	1:A:187:LYS:HB2	2.18	0.44
1:B:292:ASP:C	1:B:294:THR:H	2.25	0.44
1:B:318:VAL:O	1:B:548:THR:HA	2.17	0.44
2:F:416:PHE:N	2:F:416:PHE:HD1	2.04	0.44
1:A:589:GLU:N	1:A:590:PRO:CD	2.80	0.44
1:B:203:TRP:C	1:B:205:GLY:N	2.75	0.44
1:B:333:LEU:N	1:B:333:LEU:HD22	2.32	0.44
1:B:41:TYR:CD1	1:B:353:LYS:HG3	2.52	0.44
1:B:39:LEU:HD12	1:B:72:PHE:CD2	2.53	0.44
1:B:385:TYR:C	1:B:385:TYR:CD2	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HD23	1:A:564:GLU:HB2	2.00	0.43
1:B:146:PRO:O	1:B:150:GLU:HB2	2.18	0.43
1:B:207:TYR:CE1	1:B:398:GLU:OE2	2.71	0.43
1:B:434:THR:OG1	1:B:435:GLU:N	2.50	0.43
1:A:556:ASN:O	1:A:560:LEU:CD1	2.64	0.43
1:B:229:THR:OG1	1:B:581:VAL:HB	2.17	0.43
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.77	0.43
1:A:349:TRP:HB3	1:A:351:LEU:HD12	1.99	0.43
1:B:335:ASP:HB2	1:B:361:CYS:HB3	2.01	0.43
2:E:459:PRO:CB	2:E:467:CYS:HB3	2.48	0.43
2:E:489:ILE:C	2:E:491:TYR:H	2.26	0.43
1:A:231:GLU:C	1:A:233:ILE:H	2.27	0.43
1:A:293:VAL:HB	1:A:296:ALA:HB3	2.00	0.43
1:B:222:LEU:HD12	1:B:222:LEU:HA	1.82	0.43
2:F:365:LYS:HB3	2:F:367:TYR:CE2	2.52	0.43
1:A:90:ASN:HB3	1:A:93:VAL:HG22	2.01	0.43
1:A:174:LYS:HZ1	1:A:496:THR:HG21	1.83	0.43
1:B:30:GLU:O	1:B:34:TYR:HD1	2.01	0.43
1:B:180:TYR:O	1:B:184:VAL:HG23	2.19	0.43
1:B:414:THR:O	1:B:418:LEU:CD2	2.66	0.43
2:E:428:ILE:HG22	2:E:429:ASP:CG	2.44	0.43
1:A:532:ALA:C	1:A:534:LYS:H	2.26	0.43
2:F:361:PHE:HE2	2:F:421:LEU:HD23	1.74	0.43
1:A:130:GLY:HA3	1:A:172:VAL:HG11	2.00	0.43
1:A:560:LEU:O	1:A:561:GLY:C	2.61	0.43
1:B:226:VAL:O	1:B:229:THR:CG2	2.66	0.43
1:B:385:TYR:C	1:B:385:TYR:HD2	2.27	0.43
2:E:325:PHE:C	2:E:327:GLU:N	2.77	0.43
1:A:474:MET:HE1	1:A:499:ASP:H	1.83	0.42
1:B:407:ILE:HG23	1:B:526:GLN:NE2	2.34	0.42
1:A:126:ILE:O	1:A:130:GLY:N	2.51	0.42
1:A:367:ASP:O	1:A:371:THR:HB	2.19	0.42
1:A:599:ASN:HA	1:A:602:SER:OG	2.19	0.42
2:E:412:LEU:HD12	2:E:412:LEU:HA	1.88	0.42
1:A:229:THR:OG1	1:A:520:LEU:HD21	2.19	0.42
1:B:302:TRP:HH2	1:B:421:ILE:HG21	1.84	0.42
1:B:306:ARG:HH11	1:B:306:ARG:HG2	1.83	0.42
1:B:557:MET:HG2	1:B:573:VAL:HG11	2.00	0.42
2:F:469:PRO:HD3	2:F:474:CYS:HB3	2.01	0.42
1:A:249:MET:O	1:A:253:PRO:HA	2.20	0.42
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD12	1:A:456:LEU:C	2.45	0.42
1:B:297:MET:HE1	1:B:365:THR:O	2.19	0.42
1:A:389:PRO:HG2	1:A:392:LEU:HD22	2.02	0.42
1:A:429:GLN:H	1:A:429:GLN:CD	2.27	0.42
1:B:463:VAL:HG12	1:B:463:VAL:O	2.20	0.42
1:A:108:LEU:HD13	1:A:112:LYS:HB3	2.02	0.42
1:B:24:LEU:HD22	2:F:473:ASN:OD1	2.19	0.42
1:B:519:THR:O	1:B:522:GLN:HB3	2.20	0.42
2:E:416:PHE:N	2:E:416:PHE:HD1	2.15	0.42
1:A:198:ASP:CG	1:A:465:LYS:HG2	2.45	0.42
1:A:298:VAL:C	1:A:300:GLN:H	2.28	0.42
1:B:203:TRP:C	1:B:205:GLY:H	2.26	0.42
1:B:407:ILE:CB	1:B:408:MET:HE2	2.49	0.42
1:B:96:GLN:HB2	1:B:391:LEU:HD12	2.02	0.42
2:E:337:VAL:O	2:E:340:TRP:HD1	2.02	0.42
1:A:47:SER:HA	1:A:62:MET:CG	2.46	0.42
1:B:434:THR:O	1:B:437:ASN:HB2	2.19	0.42
2:E:448:LEU:HB3	2:E:452:GLU:HB3	2.01	0.42
2:F:405:ILE:O	2:F:409:ASN:HB2	2.19	0.42
2:F:413:PRO:HG3	2:F:451:PHE:CE1	2.55	0.42
1:A:137:ASN:C	1:A:139:GLN:H	2.28	0.41
1:A:162:LEU:HD13	1:A:490:PRO:HB2	2.02	0.41
1:A:291:ILE:HG22	1:A:291:ILE:O	2.19	0.41
1:A:425:SER:O	1:A:427:ASP:N	2.48	0.41
1:B:419:LYS:O	1:B:420:SER:C	2.62	0.41
1:B:462:MET:C	1:B:464:PHE:H	2.27	0.41
1:A:97:LEU:HG	1:A:101:GLN:HE21	1.86	0.41
1:A:184:VAL:HG13	1:A:464:PHE:CD1	2.56	0.41
1:B:425:SER:HA	1:B:426:PRO:HD2	1.87	0.41
2:F:332:THR:HG23	2:F:333:LYS:HE3	2.01	0.41
2:F:366:CYS:HA	2:F:419:CYS:HA	2.01	0.41
1:A:90:ASN:O	1:A:91:LEU:C	2.62	0.41
1:B:557:MET:CE	1:B:558:LEU:HD12	2.50	0.41
1:A:168:TRP:NE1	1:A:502:SER:HB2	2.36	0.41
1:A:231:GLU:OE2	1:A:234:LYS:HE2	2.20	0.41
1:A:456:LEU:HD12	1:A:456:LEU:O	2.20	0.41
1:A:557:MET:C	1:A:557:MET:SD	3.04	0.41
1:A:48:TRP:CE2	1:A:52:THR:HG21	2.56	0.41
1:A:256:ILE:CG2	1:A:257:SER:N	2.83	0.41
1:B:37:GLN:NE2	1:B:393:ARG:HH22	2.17	0.41
1:B:122:THR:HG22	1:B:126:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ILE:HG22	1:B:383:MET:HE3	2.02	0.41
1:B:427:ASP:O	1:B:428:PHE:C	2.63	0.41
1:B:499:ASP:HB3	5:B:902:CL:CL	2.57	0.41
1:A:488:VAL:HG21	1:A:612:PRO:HD3	2.03	0.41
1:B:324:THR:O	1:B:325:GLN:C	2.64	0.41
1:A:39:LEU:HD12	1:A:72:PHE:CD2	2.56	0.41
1:B:279:TYR:CE1	1:B:441:LYS:HB2	2.56	0.41
1:B:296:ALA:O	1:B:300:GLN:HG3	2.21	0.41
2:F:461:SER:HB2	2:F:467:CYS:SG	2.60	0.41
1:A:54:ILE:HG13	1:A:341:LYS:O	2.20	0.41
1:A:526:GLN:O	1:A:530:CYS:SG	2.79	0.41
1:B:116:LEU:HD13	1:B:186:LEU:HB2	2.03	0.41
1:B:412:ALA:HA	1:B:417:HIS:CD2	2.56	0.41
1:A:269:ASP:OD2	1:A:272:GLY:N	2.47	0.41
1:A:554:LEU:HG	1:A:558:LEU:HD22	2.03	0.41
1:B:27:THR:HG23	2:F:443:LEU:HD21	2.03	0.41
1:B:70:SER:HA	1:B:73:LEU:HD12	2.03	0.41
1:B:431:ASP:OD2	1:B:431:ASP:C	2.63	0.41
1:B:594:TRP:CZ2	1:B:598:GLN:HG3	2.56	0.41
2:F:386:SER:O	2:F:387:PHE:HB3	2.21	0.41
1:A:144:LEU:HB2	1:A:168:TRP:CH2	2.56	0.41
1:A:174:LYS:NZ	1:A:496:THR:HG23	2.36	0.41
1:A:270:MET:HB3	1:A:271:TRP:CZ3	2.56	0.41
1:A:417:HIS:HB2	1:A:543:ASP:OD2	2.20	0.41
1:B:419:LYS:HG2	1:B:424:LEU:HB3	2.03	0.41
1:B:371:THR:O	1:B:372:ALA:C	2.63	0.40
1:B:439:LEU:HD12	1:B:439:LEU:HA	1.94	0.40
1:A:174:LYS:NZ	1:A:496:THR:HG21	2.36	0.40
1:A:457:GLU:HG2	1:A:512:PHE:HB3	2.03	0.40
1:A:494:ASP:CG	1:A:496:THR:HG22	2.46	0.40
2:E:403:GLY:HA3	2:E:407:ASP:OD2	2.21	0.40
1:A:213:ASP:C	1:A:215:TYR:H	2.28	0.40
1:A:499:ASP:O	1:A:500:PRO:C	2.60	0.40
1:B:468:ILE:HA	1:B:469:PRO:HD3	1.78	0.40
1:A:288:LYS:HD2	1:A:288:LYS:HA	1.83	0.40
1:B:271:TRP:HE1	1:B:502:SER:C	2.29	0.40
1:B:278:LEU:HA	1:B:278:LEU:HD23	1.80	0.40
1:B:374:HIS:CD2	1:B:374:HIS:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	595/597 (100%)	511 (86%)	68 (11%)	16 (3%)	4	20
1	B	595/597 (100%)	509 (86%)	75 (13%)	11 (2%)	6	28
2	E	169/179 (94%)	135 (80%)	24 (14%)	10 (6%)	1	8
2	F	169/179 (94%)	135 (80%)	27 (16%)	7 (4%)	2	13
All	All	1528/1552 (98%)	1290 (84%)	194 (13%)	44 (3%)	3	19

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	PRO
1	A	504	PHE
1	B	212	VAL
1	B	290	ASN
1	B	536	GLU
2	E	330	ASN
2	E	369	VAL
2	E	402	THR
2	F	330	ASN
2	F	402	THR
1	A	91	LEU
1	A	212	VAL
1	B	91	LEU
1	B	126	ILE
1	B	163	TRP
1	B	463	VAL
1	B	473	TRP
2	E	370	SER
2	E	471	ALA
1	A	20	THR
1	A	338	ASN
1	B	322	ASN

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Mol	Chain	Res	Type
2	E	364	PHE
2	E	368	GLY
2	E	416	PHE
1	A	163	TRP
1	A	339	VAL
1	A	466	GLY
1	A	508	ASN
1	B	339	VAL
2	F	416	PHE
2	F	465	LYS
2	F	470	PRO
1	A	254	SER
1	A	505	HIS
1	A	600	LYS
1	A	614	ALA
1	B	338	ASN
1	A	409	SER
1	A	534	LYS
2	F	368	GLY
2	F	387	PHE
2	E	465	LYS
2	E	470	PRO

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	527/527 (100%)	476 (90%)	51 (10%)	8	30
1	B	527/527 (100%)	474 (90%)	53 (10%)	7	28
2	E	151/157 (96%)	136 (90%)	15 (10%)	7	29
2	F	151/157 (96%)	135 (89%)	16 (11%)	6	26
All	All	1356/1368 (99%)	1221 (90%)	135 (10%)	7	29

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	23	GLU
1	A	29	LEU
1	A	54	ILE
1	A	81	GLN
1	A	89	GLN
1	A	96	GLN
1	A	100	LEU
1	A	102	GLN
1	A	114	LYS
1	A	143	LEU
1	A	148	LEU
1	A	149	ASN
1	A	156	LEU
1	A	198	ASP
1	A	212	VAL
1	A	240	LEU
1	A	244	VAL
1	A	283	VAL
1	A	288	LYS
1	A	290	ASN
1	A	333	LEU
1	A	334	THR
1	A	364	VAL
1	A	365	THR
1	A	371	THR
1	A	380	GLN
1	A	385	TYR
1	A	410	LEU
1	A	418	LEU
1	A	429	GLN
1	A	439	LEU
1	A	444	LEU
1	A	445	THR
1	A	449	THR
1	A	456	LEU
1	A	476	LYS
1	A	479	GLU
1	A	480	MET
1	A	503	LEU
1	A	518	ARG
1	A	524	GLN
1	A	526	GLN

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Mol	Chain	Res	Type
1	A	529	LEU
1	A	536	GLU
1	A	558	LEU
1	A	560	LEU
1	A	582	ARG
1	A	597	ASP
1	A	600	LYS
1	A	607	SER
1	B	20	THR
1	B	29	LEU
1	B	47	SER
1	B	54	ILE
1	B	55	THR
1	B	70	SER
1	B	81	GLN
1	B	86	GLN
1	B	96	GLN
1	B	100	LEU
1	B	103	ASN
1	B	114	LYS
1	B	148	LEU
1	B	150	GLU
1	B	156	LEU
1	B	167	SER
1	B	170	SER
1	B	172	VAL
1	B	198	ASP
1	B	212	VAL
1	B	240	LEU
1	B	244	VAL
1	B	254	SER
1	B	290	ASN
1	B	334	THR
1	B	365	THR
1	B	367	ASP
1	B	368	ASP
1	B	369	PHE
1	B	371	THR
1	B	380	GLN
1	B	385	TYR
1	B	401	HIS
1	B	410	LEU

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Mol	Chain	Res	Type
1	B	418	LEU
1	B	432	ASN
1	B	439	LEU
1	B	444	LEU
1	B	455	MET
1	B	456	LEU
1	B	476	LYS
1	B	479	GLU
1	B	480	MET
1	B	488	VAL
1	B	502	SER
1	B	503	LEU
1	B	511	SER
1	B	527	GLU
1	B	557	MET
1	B	558	LEU
1	B	560	LEU
1	B	573	VAL
1	B	585	LEU
2	E	329	PHE
2	E	332	THR
2	E	333	LYS
2	E	337	VAL
2	E	341	GLU
2	E	359	THR
2	E	369	VAL
2	E	412	LEU
2	E	416	PHE
2	E	417	MET
2	E	428	ILE
2	E	456	SER
2	E	467	CYS
2	E	481	TYR
2	E	485	THR
2	F	329	PHE
2	F	332	THR
2	F	333	LYS
2	F	337	VAL
2	F	341	GLU
2	F	349	VAL
2	F	369	VAL
2	F	388	VAL

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Mol	Chain	Res	Type
2	F	412	LEU
2	F	416	PHE
2	F	417	MET
2	F	428	ILE
2	F	456	SER
2	F	467	CYS
2	F	485	THR
2	F	500	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	37	GLN
1	A	49	ASN
1	A	51	ASN
1	A	61	ASN
1	A	81	GLN
1	A	90	ASN
1	A	101	GLN
1	A	103	ASN
1	A	149	ASN
1	A	154	ASN
1	A	277	ASN
1	A	287	GLN
1	A	290	ASN
1	A	322	ASN
1	A	330	ASN
1	A	429	GLN
1	A	493	HIS
1	A	505	HIS
1	A	508	ASN
1	A	526	GLN
1	A	546	ASN
1	A	552	GLN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	37	GLN
1	B	42	GLN
1	B	49	ASN
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	101	GLN
1	B	103	ASN
1	B	117	ASN
1	B	121	ASN
1	B	134	ASN
1	B	137	ASN
1	B	149	ASN
1	B	154	ASN
1	B	194	ASN
1	B	221	GLN
1	B	277	ASN
1	B	290	ASN
1	B	300	GLN
1	B	322	ASN
1	B	330	ASN
1	B	340	GLN
1	B	417	HIS
1	B	493	HIS
1	B	505	HIS
1	B	524	GLN
1	B	526	GLN
1	B	546	ASN
1	B	552	GLN
1	B	556	ASN
1	B	580	ASN
1	B	586	ASN
1	B	599	ASN
1	B	601	ASN
2	E	445	HIS
2	F	357	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	NDG	B	618	-	15,15,15	0.58	0	21,21,21	1.79	5 (23%)
3	NDG	B	617	-	15,15,15	0.93	1 (6%)	21,21,21	1.85	3 (14%)
6	NAG	E	91	-	15,15,15	0.68	0	21,21,21	1.14	2 (9%)
3	NDG	B	616	-	15,15,15	0.42	0	21,21,21	1.14	3 (14%)
3	NDG	F	91	-	15,15,15	0.59	0	21,21,21	1.11	3 (14%)
3	NDG	A	616	-	15,15,15	0.63	0	21,21,21	1.05	2 (9%)

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	NDG	B	618	-	-	4/6/26/26	0/1/1/1
3	NDG	B	617	-	-	4/6/26/26	0/1/1/1
6	NAG	E	91	-	-	2/6/26/26	0/1/1/1
3	NDG	B	616	-	-	4/6/26/26	0/1/1/1
3	NDG	F	91	-	-	4/6/26/26	0/1/1/1
3	NDG	A	616	-	-	5/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	617	NDG	C1-C2	2.23	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	617	NDG	O5-C1-C2	6.35	115.90	109.52
3	B	618	NDG	O5-C1-C2	4.02	113.55	109.52
3	B	618	NDG	C1-O5-C5	3.30	120.04	113.65
6	E	91	NAG	O5-C1-C2	3.11	112.64	109.52
3	B	618	NDG	O5-C5-C4	3.09	115.26	109.70
3	A	616	NDG	C1-C2-N2	3.04	114.25	110.73
3	B	618	NDG	C1-C2-C3	2.88	114.47	110.54
3	B	618	NDG	C4-C3-C2	2.75	114.41	110.40
3	B	616	NDG	O5-C5-C4	2.73	114.62	109.70
3	B	617	NDG	C1-O5-C5	2.73	118.94	113.65
6	E	91	NAG	C1-O5-C5	2.63	118.73	113.65
3	B	617	NDG	O4-C4-C5	2.42	115.29	109.32
3	B	616	NDG	C1-O5-C5	2.28	118.06	113.65
3	F	91	NDG	O5-C1-C2	2.27	111.80	109.52
3	B	616	NDG	C3-C4-C5	2.25	114.32	110.23
3	F	91	NDG	C4-C3-C2	2.20	113.61	110.40
3	F	91	NDG	C1-O5-C5	2.14	117.79	113.65
3	A	616	NDG	C2-N2-C7	2.03	127.85	123.11

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	616	NDG	C1-C2-N2-C7
3	A	616	NDG	C8-C7-N2-C2
3	A	616	NDG	O7-C7-N2-C2
3	B	616	NDG	C8-C7-N2-C2
3	B	616	NDG	O7-C7-N2-C2
3	B	617	NDG	C8-C7-N2-C2
3	B	617	NDG	O7-C7-N2-C2
3	F	91	NDG	C8-C7-N2-C2
3	F	91	NDG	O7-C7-N2-C2
6	E	91	NAG	C8-C7-N2-C2
6	E	91	NAG	O7-C7-N2-C2
3	B	617	NDG	O5-C5-C6-O6
3	F	91	NDG	C4-C5-C6-O6
3	B	617	NDG	C4-C5-C6-O6
3	B	618	NDG	O5-C5-C6-O6
3	F	91	NDG	O5-C5-C6-O6
3	B	618	NDG	C8-C7-N2-C2
3	B	618	NDG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	616	NDG	O5-C5-C6-O6
3	B	618	NDG	O7-C7-N2-C2
3	B	616	NDG	C4-C5-C6-O6
3	B	616	NDG	O5-C5-C6-O6
3	A	616	NDG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	618	NDG	2	0
3	B	617	NDG	1	0
3	A	616	NDG	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	597/597 (100%)	-0.02	3 (0%) 87 73	37, 71, 118, 142	0
1	B	597/597 (100%)	-0.19	2 (0%) 90 80	31, 67, 116, 143	0
2	E	173/179 (96%)	0.14	1 (0%) 85 70	53, 78, 116, 120	0
2	F	173/179 (96%)	0.18	1 (0%) 85 70	54, 79, 115, 119	0
All	All	1540/1552 (99%)	-0.05	7 (0%) 87 73	31, 72, 116, 143	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	374	LEU	2.5
1	B	429	GLN	2.5
1	A	298	VAL	2.2
1	A	105	SER	2.1
2	E	415	ASP	2.1
1	A	138	PRO	2.1
1	B	85	LEU	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 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
6	NAG	E	91	15/15	0.47	0.13	147,148,148,148	0
3	NDG	F	91	15/15	0.56	0.12	117,118,118,118	0
3	NDG	B	617	15/15	0.68	0.12	98,102,103,104	0
3	NDG	B	616	15/15	0.76	0.11	105,107,108,108	0
3	NDG	A	616	15/15	0.78	0.12	114,120,121,121	0
3	NDG	B	618	15/15	0.82	0.09	56,63,70,70	0
5	CL	A	902	1/1	0.92	0.14	78,78,78,78	0
4	ZN	A	901	1/1	0.93	0.07	102,102,102,102	0
5	CL	B	902	1/1	0.95	0.12	52,52,52,52	0
4	ZN	B	901	1/1	0.95	0.05	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.