Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:22 PM EDT

PDB ID	:	3D0H
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 (i) 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 (i)) were used in the production of this report:

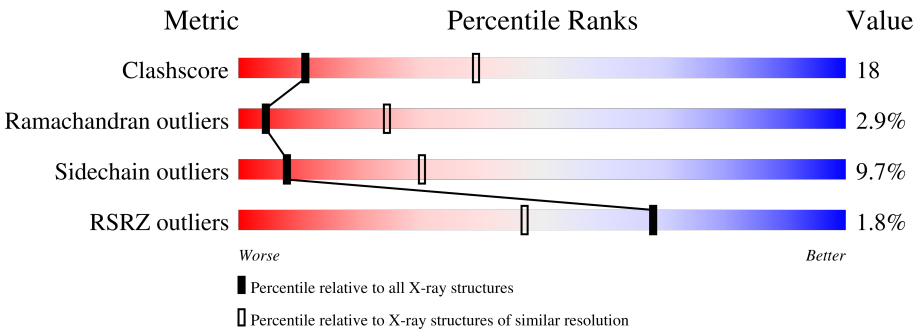
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	3%; 59%, 36%, 5%
1	B	597	%; 59%, 36%, 5%
2	E	179	2%; 61%, 25%, 9%, • •
2	F	179	%; 53%, 37%, 6%, • •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	597	4864	3110	803	922	29	0	0	0
1	B	597	4864	3110	803	922	29	0	0	0

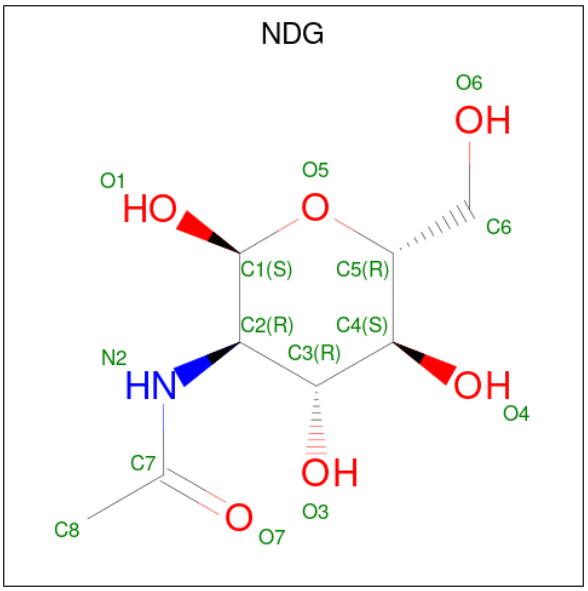
- Molecule 2 is a protein called Spike glycoprotein.

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

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-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

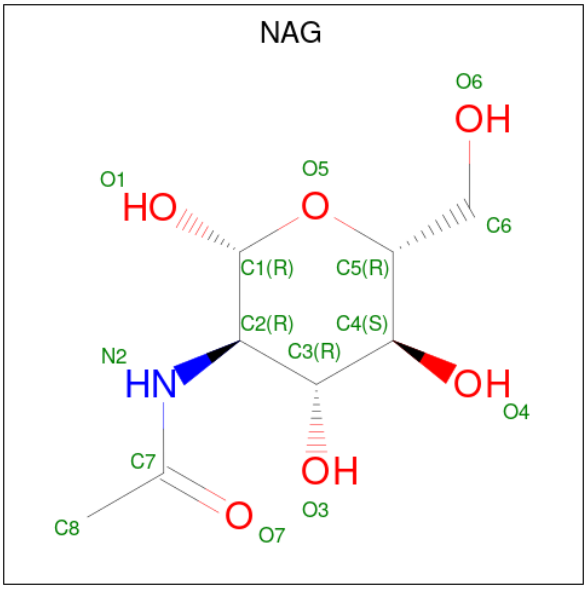
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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



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

- Molecule 7 is water.

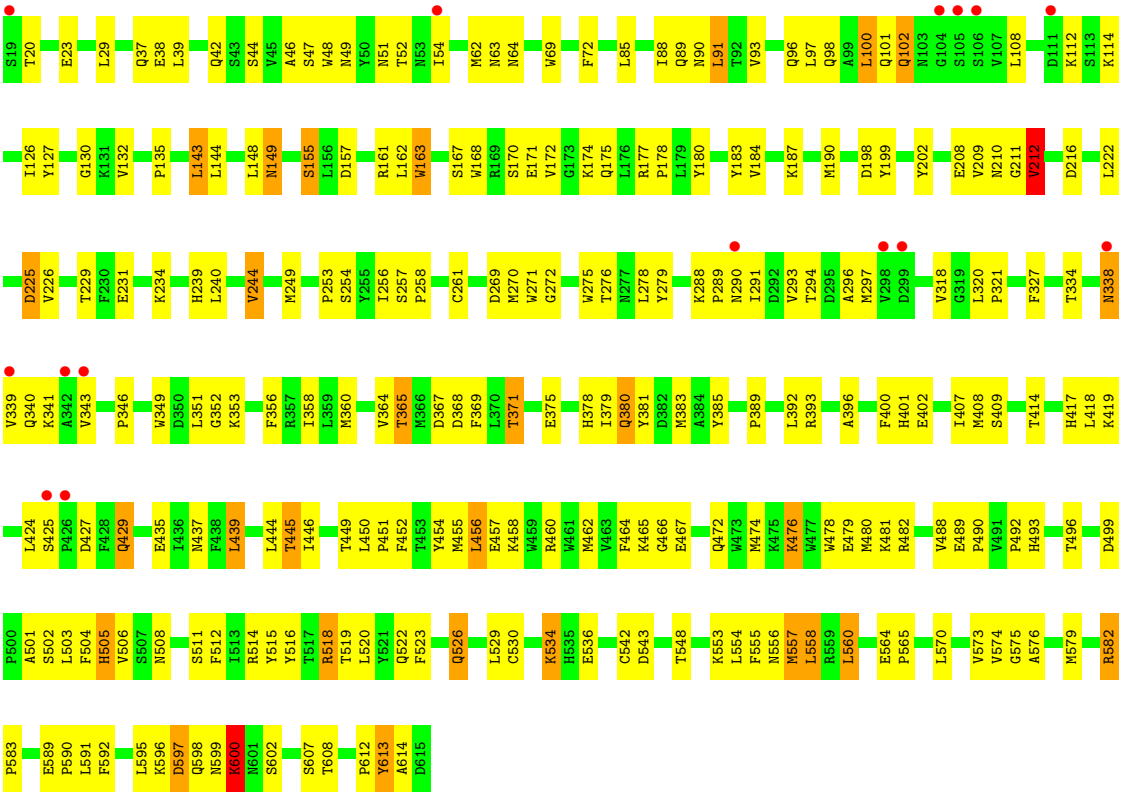
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	21	21	21	0	0
			Total	O		
7	F	6	6	6	0	0

3 Residue-property plots (i)

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

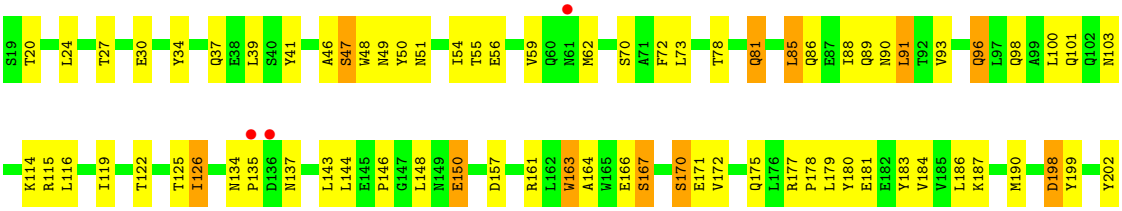
• Molecule 1: Angiotensin-converting enzyme 2

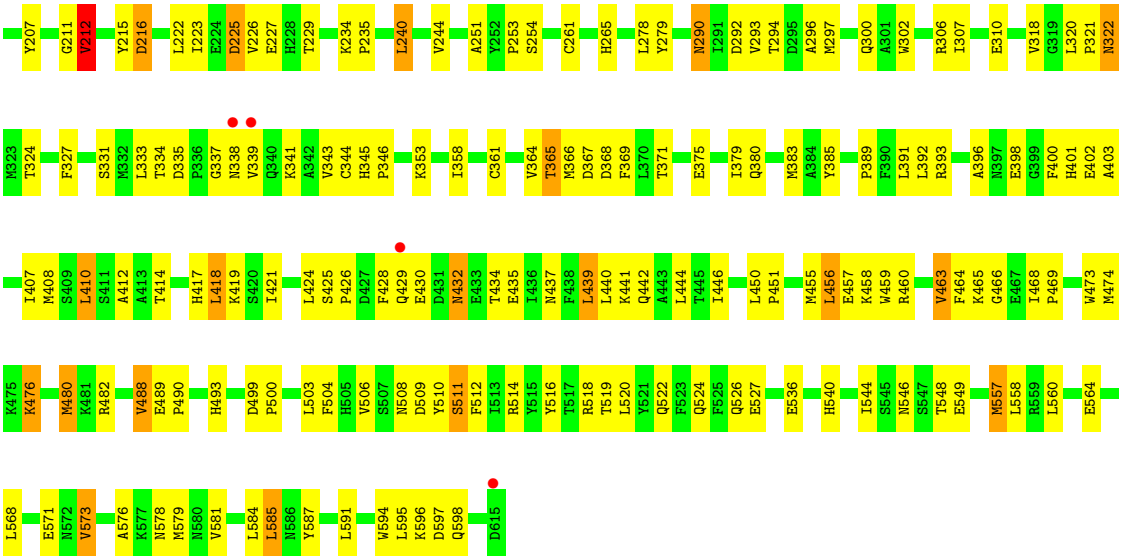
Chain A:



• Molecule 1: Angiotensin-converting enzyme 2

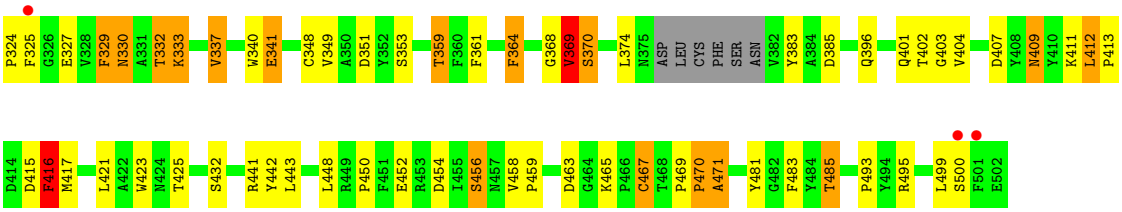
Chain B:





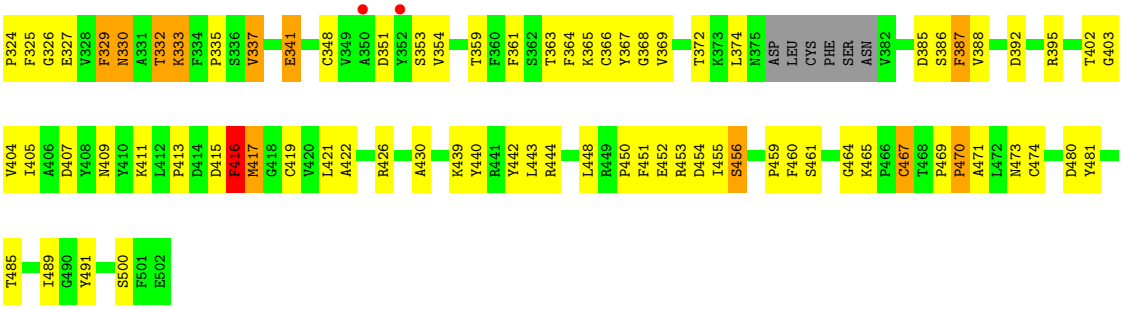
- Molecule 2: Spike glycoprotein

Chain E:



- Molecule 2: Spike glycoprotein

Chain F:



4 Data and refinement statistics (i)

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 – 3.05	Depositor EDS
% Data completeness (in resolution range)	90.3 (37.50-3.10) 87.7 (37.50-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, NAG, CL, NDG

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	0.51	0/5000	0.62	0/6796
1	B	0.55	0/5000	0.65	0/6796
2	E	0.54	0/1442	0.64	0/1961
2	F	0.55	0/1442	0.65	0/1961
All	All	0.53	0/12884	0.64	0/17514

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	4864	0	4638	170	0
1	B	4864	0	4638	175	0
2	E	1397	0	1330	43	0
2	F	1397	0	1330	62	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	446	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 18.

All (446) 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
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:51:ASN:HD22	1:B:343:VAL:HG21	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:85:LEU:HD22	1:A:101:GLN:HE22	1.57	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:455:MET:HE2	1:A:481:LYS:HG2	1.74	0.68
1:A:597:ASP:O	1:A:600:LYS:HB2	1.94	0.67
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: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
1:B:549:GLU:CD	1:B:549:GLU:H	2.00	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:E:351:ASP:C	2:E:353:SER:H	2.06	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: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: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:324:THR:O	1:B:327:PHE:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:469:PRO:HA	2:E:471:ALA:N	2.20	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
1:B:407:ILE:HB	1:B:408:MET:HE2	1.87	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: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: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: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:446:ILE:HG21	1:A:523:PHE:HE2	1.73	0.54
1:B:464:PHE:C	1:B:466:GLY:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ARG:HD3	1:A:608:THR:O	2.08	0.53
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:482:ARG:HG2	1:B:488:VAL:CG1	2.39	0.53
1:A:135:PRO:CD	1:A:163:TRP:HE1	2.22	0.53
1:A:407:ILE:HB	1:A:408:MET:HE2	1.91	0.53
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:183:TYR:O	1:B:187:LYS:HB2	2.09	0.52
2:F:469:PRO:HA	2:F:471:ALA:N	2.25	0.52
1:B:51:ASN:HD22	1:B:343:VAL:CG2	2.23	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: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:B:474:MET:CE	1:B:499:ASP:H	2.23	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
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
1:A:85:LEU:HA	1:A:88:ILE:HD12	1.93	0.51
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:F:403:GLY:HA2	2:F:407:ASP:CG	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:504:PHE:C	1:B:504:PHE:CD2	2.85	0.50
1:A:256:ILE:HG22	1:A:257:SER:N	2.26	0.50
1:A:352:GLY:O	1:A:353:LYS:C	2.49	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: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: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
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:63:ASN:O	1:A:64:ASN:C	2.50	0.49
1:A:501:ALA:HA	1:A:506:VAL:HG11	1.93	0.49
2:E:442:TYR:HD1	2:E:443:LEU:HG	1.75	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
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: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:546:ASN:ND2	3:B:618:NDG:C1	2.73	0.49
1:B:557:MET:HE2	1:B:558:LEU:HD12	1.94	0.49
2:E:325:PHE:C	2:E:327:GLU:H	2.15	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:B:167:SER:O	1:B:171:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:HIS:CE1	1:A:515:TYR:HE2	2.31	0.48
1:B:464:PHE:C	1:B:466:GLY:N	2.66	0.48
1:A:249:MET:HE3	1:A:258:PRO:N	2.28	0.48
1:B:578:ASN:CG	1:B:579:MET:H	2.17	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
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
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: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
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:A:100:LEU:C	1:A:102:GLN:H	2.18	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
2:E:359:THR:C	2:E:361:PHE:H	2.18	0.47
2:E:469:PRO:HA	2:E:470:PRO:C	2.35	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:297:MET:CE	1:B:307:ILE:HD11	2.45	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:F:359:THR:C	2:F:361:PHE:H	2.18	0.46
1:A:261:CYS:CB	1:A:488:VAL:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:TYR:CD2	2:F:440:TYR:OH	2.66	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:A:474:MET:CE	1:A:499:ASP:H	2.28	0.46
1:B:229:THR:OG1	1:B:520:LEU:HD21	2.16	0.46
1:B:251:ALA:C	1:B:253:PRO:HD3	2.35	0.46
2:E:396:GLN:HA	2:E:401:GLN:HG3	1.97	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
2:F:461:SER:HB3	2:F:464:GLY:O	2.16	0.45
1:A:505:HIS:CE1	1:A:515:TYR:CE2	3.04	0.45
1:B:578:ASN:CG	1:B:579:MET:N	2.70	0.45
1:A:321:PRO:HD2	1:A:380:GLN:OE1	2.16	0.45
1:B:335:ASP:C	1:B:337:GLY:H	2.20	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:A:209:VAL:HG21	1:A:565:PRO:HB3	1.98	0.45
1:A:435:GLU:O	1:A:439:LEU:HD22	2.17	0.45
1:B:489:GLU:CD	1:B:489:GLU:H	2.19	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:429:GLN:CD	1:B:429:GLN:H	2.20	0.45
2:E:415:ASP:O	2:E:416:PHE:C	2.54	0.45
2:F:337:VAL:CG1	2:F:387:PHE:CD1	3.00	0.45
1:B:198:ASP:CG	1:B:465:LYS:HG2	2.37	0.45
2:E:369:VAL:HB	2:E:370:SER:H	1.42	0.45
2:F:325:PHE:C	2:F:327:GLU:H	2.19	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:A:454:TYR:CD2	1:A:454:TYR:C	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:MET:HE2	1:A:499:ASP:H	1.82	0.44
1:B:78:THR:O	1:B:81:GLN:HB2	2.18	0.44
1:A:175:GLN:O	1:A:178:PRO:HD2	2.17	0.44
2:F:415:ASP:O	2:F:416:PHE:C	2.54	0.44
1:A:46:ALA:O	1:A:47:SER:C	2.56	0.44
1:A:135:PRO:CD	1:A:163:TRP:NE1	2.80	0.44
1:A:452:PHE:CD1	1:A:452:PHE:C	2.90	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:163:TRP:O	1:B:164:ALA:C	2.56	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: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:A:425:SER:C	1:A:427:ASP:H	2.21	0.44
1:B:39:LEU:HD12	1:B:72:PHE:CD2	2.53	0.44
1:B:344:CYS:O	1:B:345:HIS:C	2.56	0.44
1:A:458:LYS:O	1:A:462:MET:HE2	2.19	0.43
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:297:MET:HE1	1:B:307:ILE:HD11	2.00	0.43
1:B:335:ASP:HB2	1:B:361:CYS:HB3	2.01	0.43
1:A:465:LYS:C	1:A:467:GLU:H	2.22	0.43
2:E:459:PRO:CB	2:E:467:CYS:HB3	2.48	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:351:ASP:C	2:F:353:SER:H	2.22	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: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:F:489:ILE:C	2:F:491:TYR:H	2.22	0.43
2:F:361:PHE:HE2	2:F:421:LEU:HD23	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLY:HA3	1:A:172:VAL:HG11	2.00	0.43
1:B:226:VAL:O	1:B:229:THR:CG2	2.66	0.43
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:222:LEU:O	1:B:223:ILE:C	2.58	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:291:ILE:HG22	1:A:291:ILE:O	2.19	0.42
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.84	0.42
1:B:544:ILE:C	1:B:544:ILE:HD12	2.40	0.42
1:A:174:LYS:HZ1	1:A:496:THR:CG2	2.32	0.42
1:A:389:PRO:HG2	1:A:392:LEU:HD22	2.02	0.42
1:B:456:LEU:C	1:B:456:LEU:CD1	2.87	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:B:366:MET:HE1	1:B:441:LYS:HE3	2.00	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:351:ASP:C	2:E:353:SER:N	2.73	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
1:A:174:LYS:HZ1	1:A:496:THR:HG21	1.84	0.42
1:A:297:MET:HE2	1:A:364:VAL:HG12	2.02	0.42
2:F:413:PRO:HG3	2:F:451:PHE:CE1	2.55	0.42
1:A:162:LEU:HD13	1:A:490:PRO:HB2	2.02	0.41
1:A:425:SER:O	1:A:427:ASP:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:474:MET:HE1	1:B:499:ASP:H	1.84	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: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:A:592:PHE:HE2	1:A:596:LYS:HZ2	1.69	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
1:B:211:GLY:C	1:B:212:VAL:HG22	2.40	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
2:F:469:PRO:HA	2:F:470:PRO:C	2.41	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:E:458:VAL:O	2:E:459:PRO:C	2.59	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:125:THR:O	1:B:126:ILE:C	2.58	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:594:TRP:CZ2	1:B:598:GLN:HG3	2.56	0.41
1:B:595:LEU:O	1:B:596:LYS:C	2.60	0.41
1:B:597:ASP:O	1:B:598:GLN:C	2.59	0.41
2:F:325:PHE:C	2:F:327:GLU:N	2.73	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:439:LEU:HD12	1:B:439:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:292:ASP:C	1:B:294:THR:H	2.25	0.40
2:E:403:GLY:HA3	2:E:407:ASP:OD2	2.21	0.40
1:B:143:LEU:O	1:B:144:LEU:C	2.59	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:278:LEU:HA	1:B:278:LEU:HD23	1.80	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	595/597 (100%)	511 (86%)	68 (11%)	16 (3%)	5 25
1	B	595/597 (100%)	509 (86%)	75 (13%)	11 (2%)	8 34
2	E	169/179 (94%)	135 (80%)	24 (14%)	10 (6%)	1 10
2	F	169/179 (94%)	135 (80%)	27 (16%)	7 (4%)	3 16
All	All	1528/1552 (98%)	1290 (84%)	194 (13%)	44 (3%)	4 24

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

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Mol	Chain	Res	Type
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
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 (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	527/527 (100%)	477 (90%)	50 (10%)	8 31
1	B	527/527 (100%)	479 (91%)	48 (9%)	9 33
2	E	151/157 (96%)	133 (88%)	18 (12%)	5 20
2	F	151/157 (96%)	136 (90%)	15 (10%)	8 29
All	All	1356/1368 (99%)	1225 (90%)	131 (10%)	8 30

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	29	LEU
1	A	69	TRP
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	149	ASN
1	A	155	SER
1	A	190	MET
1	A	198	ASP
1	A	212	VAL
1	A	216	ASP
1	A	225	ASP
1	A	244	VAL
1	A	290	ASN
1	A	334	THR
1	A	365	THR
1	A	368	ASP
1	A	369	PHE
1	A	371	THR
1	A	380	GLN
1	A	381	TYR
1	A	385	TYR
1	A	401	HIS
1	A	418	LEU

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Mol	Chain	Res	Type
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	526	GLN
1	A	529	LEU
1	A	536	GLU
1	A	557	MET
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	A	613	TYR
1	B	20	THR
1	B	47	SER
1	B	55	THR
1	B	81	GLN
1	B	85	LEU
1	B	86	GLN
1	B	89	GLN
1	B	96	GLN
1	B	100	LEU
1	B	103	ASN
1	B	114	LYS
1	B	150	GLU
1	B	167	SER
1	B	170	SER
1	B	172	VAL
1	B	190	MET
1	B	198	ASP
1	B	212	VAL
1	B	216	ASP
1	B	225	ASP

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Mol	Chain	Res	Type
1	B	240	LEU
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	385	TYR
1	B	401	HIS
1	B	410	LEU
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	480	MET
1	B	488	VAL
1	B	503	LEU
1	B	511	SER
1	B	527	GLU
1	B	557	MET
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	364	PHE
2	E	369	VAL
2	E	409	ASN
2	E	412	LEU
2	E	416	PHE
2	E	417	MET
2	E	423	TRP
2	E	456	SER

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Mol	Chain	Res	Type
2	E	463	ASP
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	364	PHE
2	F	369	VAL
2	F	388	VAL
2	F	416	PHE
2	F	417	MET
2	F	456	SER
2	F	467	CYS
2	F	481	TYR
2	F	485	THR
2	F	500	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) 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	90	ASN
1	A	96	GLN
1	A	101	GLN
1	A	149	ASN
1	A	194	ASN
1	A	277	ASN
1	A	287	GLN
1	A	290	ASN
1	A	429	GLN
1	A	493	HIS
1	A	505	HIS
1	A	526	GLN
1	A	546	ASN
1	A	586	ASN
1	B	33	ASN

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	49	ASN
1	B	51	ASN
1	B	64	ASN
1	B	96	GLN
1	B	101	GLN
1	B	149	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	325	GLN
1	B	330	ASN
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	580	ASN
1	B	586	ASN
1	B	601	ASN
2	E	445	HIS
2	F	375	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 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	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	A	616	-	15,15,15	0.63	0	21,21,21	1.05	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	B	618	-	15,15,15	0.58	0	21,21,21	1.79	5 (23%)

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	617	-	-	4/6/26/26	0/1/1/1
6	NAG	E	91	-	-	2/6/26/26	0/1/1/1
3	NDG	A	616	-	-	5/6/26/26	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	B	618	-	-	4/6/26/26	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(^{o})	Ideal(^{o})
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
3	A	616	NDG	O5-C5-C6-O6
3	B	618	NDG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
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	617	NDG	1	0
3	A	616	NDG	1	0
3	B	618	NDG	2	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%)	-0.09	15 (2%)	57	34	37, 71, 118, 142	0
1	B	597/597 (100%)	-0.20	7 (1%)	79	61	31, 67, 116, 143	0
2	E	173/179 (96%)	-0.06	3 (1%)	70	49	53, 78, 116, 120	0
2	F	173/179 (96%)	-0.04	2 (1%)	79	61	54, 79, 115, 119	0
All	All	1540/1552 (99%)	-0.12	27 (1%)	68	47	31, 72, 116, 143	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	GLY	5.2
1	A	19	SER	4.8
1	A	105	SER	4.2
1	B	136	ASP	3.8
1	A	106	SER	3.7
1	B	339	VAL	3.3
1	A	290	ASN	3.1
1	B	615	ASP	3.0
1	A	342	ALA	2.8
2	E	501	PHE	2.8
1	A	298	VAL	2.7
1	A	343	VAL	2.5
1	B	338	ASN	2.4
2	F	352	TYR	2.3
1	A	299	ASP	2.3
1	B	429	GLN	2.2
1	A	111	ASP	2.1
1	B	135	PRO	2.1
2	E	500	SER	2.1
1	A	426	PRO	2.1
1	A	54	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	350	ALA	2.1
1	A	338	ASN	2.1
1	A	425	SER	2.1
1	A	339	VAL	2.0
2	E	325	PHE	2.0
1	B	61	ASN	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 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(Å^2)	Q<0.9
6	NAG	E	91	15/15	0.60	0.36	147,148,148,148	0
3	NDG	B	617	15/15	0.75	0.24	98,102,103,104	0
3	NDG	F	91	15/15	0.76	0.25	117,118,118,118	0
3	NDG	B	616	15/15	0.78	0.31	105,107,108,108	0
3	NDG	B	618	15/15	0.84	0.18	56,63,70,70	0
4	ZN	A	901	1/1	0.85	0.38	102,102,102,102	0
3	NDG	A	616	15/15	0.85	0.22	114,120,121,121	0
5	CL	A	902	1/1	0.92	0.32	78,78,78,78	0
5	CL	B	902	1/1	0.97	0.23	52,52,52,52	0
4	ZN	B	901	1/1	0.97	0.35	110,110,110,110	0

6.5 Other polymers (i)

There are no such residues in this entry.