Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:15 PM EDT

PDB ID	:	3D0G
Title	:	Crystal structure of spike protein receptor-binding domain from the 2002-2003 SARS coronavirus human strain complexed with human-civet chimeric receptor ACE2
Authors	:	Li, F.
Deposited on	:	2008-05-01
Resolution	:	2.80 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:

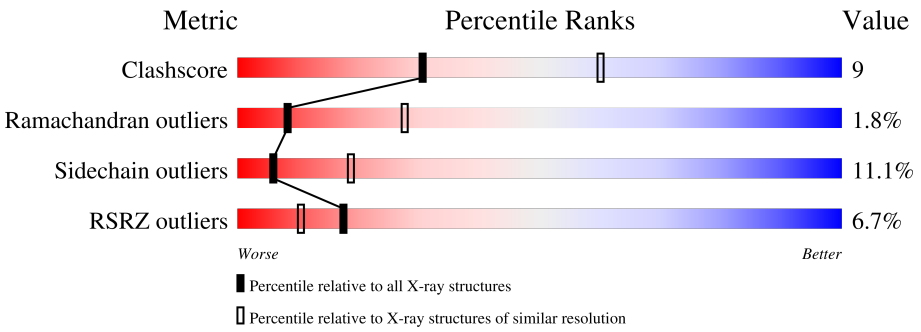
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	7% 74% 22% •
1	B	597	5% 73% 25% • •
2	E	179	13% 68% 24% • • •
2	F	179	4% 65% 26% • • •

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.

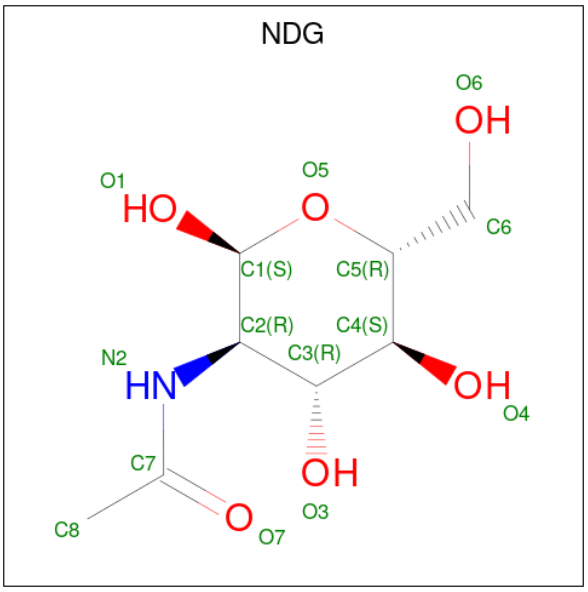
- Molecule 1 is a protein called Angiotensin-converting enzyme 2.

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	906	227	258	6	0	0	0
2	F	173	1397	906	227	258	6	0	0	0

- 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

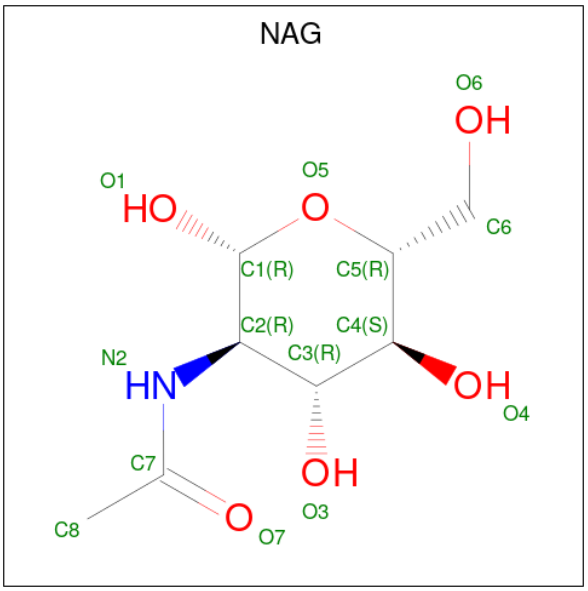
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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.

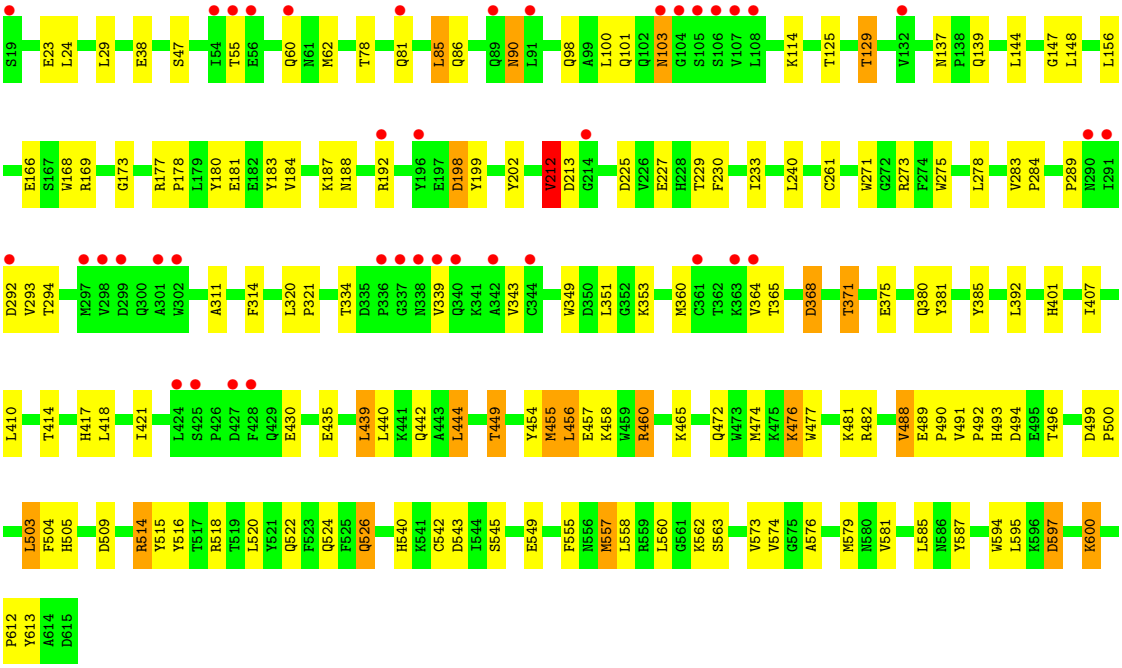
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	B	21	21	21	0	0
			Total	O		
7	F	6	6	6	0	0

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.

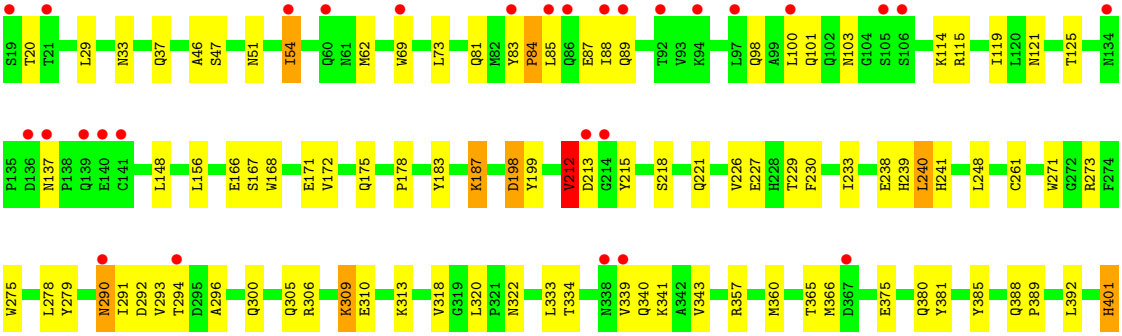
• Molecule 1: Angiotensin-converting enzyme 2

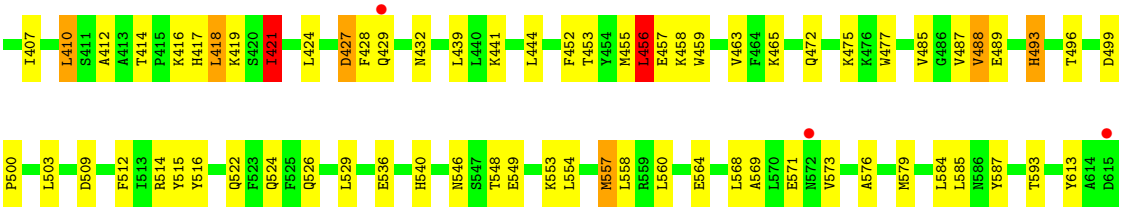
Chain A:



• Molecule 1: Angiotensin-converting enzyme 2

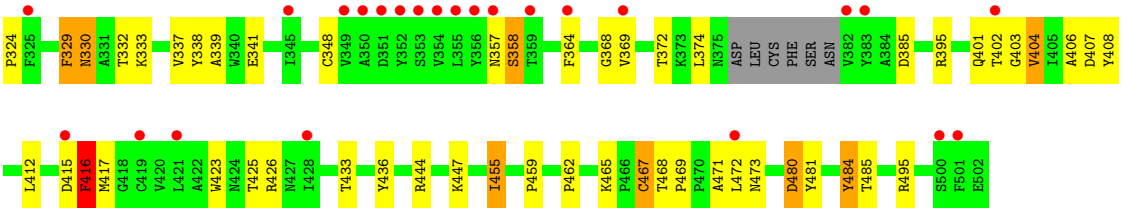
Chain B:





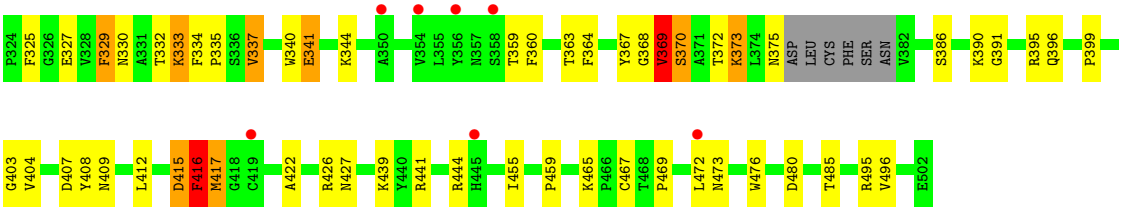
- Molecule 2: Spike glycoprotein

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	80.01Å 119.76Å 108.80Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	47.14 – 2.80 47.16 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.8 (47.14-2.80) 88.7 (47.16-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.214 , 0.279 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12643	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: NAG, ZN, 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	0.49	0/5000	0.60	0/6796
1	B	0.52	0/5000	0.63	2/6796 (0.0%)
2	E	0.52	0/1442	0.63	0/1963
2	F	0.51	0/1442	0.64	0/1963
All	All	0.51	0/12884	0.62	2/17518 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	456	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	421	ILE	CB-CA-C	-5.23	101.14	111.60

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	94	0
1	B	4864	0	4638	83	0
2	E	1397	0	1325	27	0
2	F	1397	0	1325	26	0
3	A	15	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	36	4	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	1	0
5	B	1	0	0	1	0
6	E	15	0	15	0	0
7	B	21	0	0	3	0
7	F	6	0	0	0	0
All	All	12643	0	12001	227	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 9.

All (227) 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:261:CYS:HB2	1:B:488:VAL:HG22	1.46	0.97
1:B:47:SER:HA	1:B:62:MET:HG3	1.49	0.93
1:A:524:GLN:HE22	1:A:579:MET:HA	1.35	0.91
1:A:47:SER:HA	1:A:62:MET:HG3	1.53	0.90
2:E:425:THR:HG21	2:E:495:ARG:HG3	1.58	0.84
1:A:24:LEU:HD22	2:E:473:ASN:HD22	1.45	0.81
1:A:457:GLU:OE2	1:A:460:ARG:NH1	2.16	0.78
1:A:261:CYS:CB	1:A:488:VAL:HG22	2.13	0.78
2:E:329:PHE:O	2:E:330:ASN:HB2	1.83	0.77
1:A:414:THR:HG21	1:A:542:CYS:O	1.84	0.77
2:F:459:PRO:HB2	2:F:467:CYS:HB2	1.68	0.75
1:B:407:ILE:HD11	1:B:522:GLN:O	1.86	0.75
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.70	0.73
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.69	0.73
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.71	0.72
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.72	0.72
1:B:557:MET:HE2	1:B:558:LEU:HD12	1.72	0.71
1:B:47:SER:HA	1:B:62:MET:CG	2.20	0.71
2:F:329:PHE:O	2:F:330:ASN:HB2	1.90	0.71
1:B:414:THR:O	1:B:418:LEU:HD22	1.91	0.71
2:E:404:VAL:H	2:E:407:ASP:HB2	1.57	0.70
1:B:279:TYR:CE1	1:B:441:LYS:HB2	2.26	0.70
1:B:546:ASN:HD21	3:B:618:NDG:C1	2.05	0.70
1:B:293:VAL:HG22	1:B:366:MET:HG3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LEU:HD22	1:B:477:TRP:HH2	1.57	0.69
1:A:229:THR:OG1	1:A:581:VAL:HB	1.91	0.69
1:A:430:GLU:HB3	1:A:435:GLU:OE2	1.93	0.68
1:A:85:LEU:HD22	1:A:101:GLN:HE22	1.57	0.68
1:A:229:THR:HG23	1:A:516:TYR:OH	1.95	0.67
1:B:419:LYS:HD3	1:B:428:PHE:HB3	1.76	0.67
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.77	0.65
1:A:85:LEU:H	1:A:85:LEU:HD23	1.60	0.65
2:F:408:TYR:CD2	2:F:444:ARG:HB3	2.33	0.64
1:A:230:PHE:HA	1:A:233:ILE:HD12	1.80	0.64
1:A:261:CYS:HB3	1:A:488:VAL:HG22	1.79	0.63
1:B:273:ARG:HG3	1:B:452:PHE:CE1	2.34	0.63
2:F:459:PRO:HB2	2:F:467:CYS:CB	2.28	0.63
1:A:225:ASP:O	1:A:229:THR:HG22	1.98	0.62
1:A:560:LEU:O	1:A:563:SER:HB3	2.00	0.61
1:B:571:GLU:HA	1:B:576:ALA:H	1.64	0.61
2:E:416:PHE:CD1	2:E:416:PHE:N	2.67	0.61
1:B:275:TRP:HB3	1:B:278:LEU:HD12	1.83	0.61
1:A:137:ASN:HD21	1:A:139:GLN:HE21	1.48	0.61
1:A:543:ASP:OD1	1:A:545:SER:HB2	2.01	0.61
1:B:54:ILE:HG22	1:B:54:ILE:O	2.01	0.60
1:A:524:GLN:NE2	1:A:579:MET:HA	2.11	0.60
2:E:469:PRO:HA	2:E:471:ALA:N	2.16	0.60
2:E:426:ARG:HD3	2:E:485:THR:HG23	1.82	0.60
1:A:417:HIS:CD2	1:A:421:ILE:HD11	2.37	0.60
1:B:564:GLU:OE1	1:B:568:LEU:HD12	2.03	0.59
1:A:198:ASP:OD1	1:A:465:LYS:HG2	2.02	0.58
1:B:226:VAL:O	1:B:229:THR:HG22	2.03	0.58
1:B:427:ASP:HB2	7:B:918:HOH:O	2.03	0.58
1:B:168:TRP:O	1:B:172:VAL:HG22	2.03	0.58
1:B:546:ASN:ND2	3:B:618:NDG:O1	2.37	0.58
1:A:166:GLU:OE1	1:A:493:HIS:HE1	1.86	0.58
1:A:180:TYR:O	1:A:184:VAL:HG23	2.04	0.58
1:A:187:LYS:HG2	1:A:199:TYR:CE2	2.39	0.57
2:E:357:ASN:O	2:E:358:SER:HB2	2.02	0.57
1:A:557:MET:HA	1:A:560:LEU:HD12	1.86	0.57
1:A:560:LEU:O	1:A:563:SER:CB	2.52	0.57
1:B:183:TYR:OH	1:B:509:ASP:OD1	2.16	0.57
1:A:494:ASP:OD2	1:A:496:THR:HG22	2.06	0.56
1:A:320:LEU:HB3	1:A:321:PRO:HD2	1.88	0.56
1:A:125:THR:O	1:A:129:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD13	1:A:444:LEU:HD22	1.87	0.56
1:B:293:VAL:CG2	1:B:366:MET:HG3	2.36	0.56
1:A:294:THR:HG23	1:A:365:THR:HA	1.87	0.55
1:B:46:ALA:HB1	1:B:62:MET:HA	1.88	0.55
1:A:177:ARG:O	1:A:181:GLU:HG3	2.06	0.55
1:B:175:GLN:O	1:B:178:PRO:HD2	2.06	0.55
1:A:474:MET:HE1	1:A:499:ASP:HB2	1.89	0.55
1:B:554:LEU:HG	1:B:558:LEU:HD13	1.89	0.54
2:F:403:GLY:HA2	2:F:407:ASP:CG	2.27	0.54
1:A:183:TYR:OH	1:A:509:ASP:OD1	2.20	0.54
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.89	0.54
1:A:275:TRP:HB3	1:A:278:LEU:HD12	1.90	0.54
1:B:546:ASN:ND2	3:B:618:NDG:C1	2.71	0.54
1:A:24:LEU:HD22	2:E:473:ASN:ND2	2.21	0.53
1:A:368:ASP:HA	1:A:371:THR:HB	1.90	0.53
1:A:526:GLN:HA	1:A:526:GLN:NE2	2.24	0.53
2:E:469:PRO:HA	2:E:471:ALA:H	1.73	0.52
2:F:335:PRO:HG3	2:F:341:GLU:CG	2.38	0.52
1:A:503:LEU:HD22	1:A:504:PHE:H	1.75	0.52
1:B:218:SER:H	1:B:221:GLN:NE2	2.08	0.52
2:E:329:PHE:O	2:E:330:ASN:CB	2.57	0.52
1:A:503:LEU:HD22	1:A:504:PHE:N	2.25	0.51
1:A:183:TYR:O	1:A:187:LYS:HB2	2.10	0.51
1:B:166:GLU:OE1	1:B:493:HIS:HE1	1.94	0.51
1:A:349:TRP:HB3	1:A:351:LEU:CD1	2.41	0.51
1:A:574:VAL:HG23	1:A:576:ALA:H	1.75	0.51
1:B:296:ALA:O	1:B:300:GLN:HG3	2.11	0.51
2:F:404:VAL:H	2:F:407:ASP:HB2	1.76	0.51
1:A:407:ILE:HD11	1:A:522:GLN:O	2.11	0.50
1:A:90:ASN:C	1:A:90:ASN:HD22	2.13	0.50
2:F:334:PHE:CD2	2:F:386:SER:HB3	2.47	0.50
1:B:261:CYS:CB	1:B:488:VAL:HG22	2.29	0.49
1:B:499:ASP:HB3	5:B:902:CL:CL	2.49	0.49
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.95	0.49
1:B:294:THR:HG23	1:B:365:THR:HA	1.93	0.49
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.95	0.49
2:F:409:ASN:HD21	2:F:441:ARG:H	1.61	0.49
1:B:540:HIS:HA	1:B:587:TYR:CE1	2.47	0.48
2:F:416:PHE:CD1	2:F:416:PHE:N	2.82	0.48
1:A:557:MET:C	1:A:557:MET:SD	2.92	0.48
1:A:227:GLU:OE2	1:A:458:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:HIS:HB2	1:A:543:ASP:OD2	2.13	0.48
2:E:436:TYR:OH	2:E:484:TYR:OH	2.26	0.48
1:A:103:ASN:HD22	1:A:103:ASN:C	2.17	0.48
1:B:569:ALA:O	1:B:573:VAL:HG23	2.13	0.48
2:F:332:THR:HG23	2:F:333:LYS:HG3	1.95	0.48
1:A:360:MET:SD	1:A:371:THR:HG22	2.53	0.48
1:B:293:VAL:HG11	1:B:418:LEU:HG	1.96	0.48
1:B:318:VAL:O	1:B:548:THR:HA	2.14	0.48
1:B:401:HIS:CB	7:B:904:HOH:O	2.62	0.48
2:E:425:THR:HG21	2:E:495:ARG:CG	2.37	0.48
2:E:436:TYR:O	2:E:480:ASP:OD2	2.32	0.47
2:E:436:TYR:HH	2:E:484:TYR:HH	1.52	0.47
1:B:230:PHE:HA	1:B:233:ILE:HD12	1.97	0.47
1:A:320:LEU:HB3	1:A:321:PRO:CD	2.44	0.47
1:A:271:TRP:CE2	1:A:503:LEU:HD23	2.49	0.47
1:A:499:ASP:N	1:A:500:PRO:HD2	2.30	0.47
1:B:33:ASN:O	1:B:37:GLN:HG3	2.14	0.47
2:E:341:GLU:O	2:E:385:ASP:HA	2.15	0.47
2:F:373:LYS:HD3	2:F:375:ASN:HD22	1.79	0.47
1:B:227:GLU:OE2	1:B:458:LYS:HE2	2.15	0.47
1:A:454:TYR:CE2	1:A:458:LYS:HD3	2.50	0.47
1:A:499:ASP:HB3	5:A:902:CL:CL	2.52	0.47
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.49	0.47
1:B:417:HIS:O	1:B:421:ILE:HG13	2.15	0.46
1:B:493:HIS:HD2	1:B:499:ASP:OD1	1.99	0.46
2:F:415:ASP:O	2:F:416:PHE:C	2.53	0.46
2:F:396:GLN:OE1	2:F:403:GLY:O	2.34	0.46
1:A:98:GLN:HA	1:A:101:GLN:HE21	1.81	0.45
1:A:489:GLU:HG2	1:A:613:TYR:HE2	1.81	0.45
1:B:198:ASP:OD1	1:B:465:LYS:HG2	2.16	0.45
2:F:337:VAL:O	2:F:340:TRP:HD1	1.99	0.45
1:B:306:ARG:O	1:B:310:GLU:HB2	2.17	0.45
2:F:469:PRO:HG3	2:F:476:TRP:NE1	2.30	0.45
1:A:472:GLN:O	1:A:476:LYS:HB2	2.16	0.45
1:A:199:TYR:O	1:A:202:TYR:HB3	2.16	0.45
1:B:472:GLN:HG2	1:B:475:LYS:HE3	1.97	0.45
2:E:329:PHE:H	2:E:329:PHE:HD2	1.60	0.45
1:A:38:GLU:OE2	1:A:353:LYS:NZ	2.45	0.45
1:A:597:ASP:O	1:A:600:LYS:HB2	2.17	0.45
2:E:403:GLY:HA2	2:E:406:ALA:HB3	1.98	0.45
2:F:334:PHE:CD1	2:F:495:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:439:LYS:HD3	2:F:480:ASP:OD1	2.17	0.45
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.88	0.45
1:B:187:LYS:HG2	1:B:199:TYR:CE2	2.52	0.45
1:B:524:GLN:HE22	1:B:579:MET:HA	1.81	0.45
2:F:363:THR:HB	2:F:422:ALA:HB3	1.97	0.45
1:B:456:LEU:HD22	1:B:477:TRP:CH2	2.44	0.44
2:F:325:PHE:C	2:F:327:GLU:H	2.19	0.44
2:E:403:GLY:HA3	2:E:407:ASP:CG	2.37	0.44
1:B:85:LEU:HD22	1:B:101:GLN:HE22	1.82	0.44
1:B:47:SER:O	1:B:51:ASN:OD1	2.36	0.44
1:B:459:TRP:O	1:B:463:VAL:HG23	2.17	0.44
1:B:485:VAL:HG12	1:B:487:VAL:HG23	2.00	0.44
1:B:499:ASP:N	1:B:500:PRO:HD2	2.32	0.44
1:B:320:LEU:HB3	1:B:380:GLN:OE1	2.18	0.44
1:B:584:LEU:C	1:B:584:LEU:HD23	2.38	0.44
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.57	0.44
1:A:24:LEU:HD23	2:E:462:PRO:HG2	1.99	0.43
1:B:83:TYR:HA	1:B:84:PRO:HD2	1.85	0.43
1:B:85:LEU:HA	1:B:88:ILE:HD12	2.00	0.43
1:B:418:LEU:HB2	1:B:424:LEU:HD22	1.99	0.43
1:A:261:CYS:HB2	1:A:488:VAL:CG2	2.46	0.43
1:B:453:THR:HG23	1:B:512:PHE:CD1	2.54	0.43
1:A:273:ARG:O	1:A:449:THR:OG1	2.34	0.43
1:B:401:HIS:HB3	7:B:904:HOH:O	2.19	0.43
1:A:188:ASN:O	1:A:192:ARG:HG3	2.19	0.43
1:A:455:MET:SD	1:A:481:LYS:HG2	2.59	0.43
1:B:322:ASN:HD21	3:B:617:NDG:C1	2.32	0.43
1:A:482:ARG:HG2	1:A:488:VAL:HG13	2.01	0.43
1:B:166:GLU:OE1	1:B:493:HIS:CE1	2.71	0.43
1:A:540:HIS:HA	1:A:587:TYR:CE1	2.54	0.43
1:B:119:ILE:HG21	1:B:183:TYR:HB2	2.00	0.42
1:A:417:HIS:O	1:A:421:ILE:HG13	2.19	0.42
1:A:144:LEU:HD22	1:A:168:TRP:CZ2	2.55	0.42
1:A:169:ARG:O	1:A:173:GLY:HA3	2.19	0.42
1:A:520:LEU:O	1:A:524:GLN:HG3	2.19	0.42
1:B:69:TRP:CE2	1:B:73:LEU:HD11	2.55	0.42
1:B:238:GLU:O	1:B:241:HIS:HB3	2.19	0.42
2:F:367:TYR:HB2	2:F:417:MET:HB3	2.01	0.42
1:B:115:ARG:O	1:B:119:ILE:HG12	2.18	0.42
1:A:311:ALA:O	1:A:314:PHE:HB3	2.20	0.42
1:B:514:ARG:HG2	1:B:515:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:HD22	1:A:477:TRP:HH2	1.85	0.42
1:A:225:ASP:O	1:A:229:THR:CG2	2.64	0.42
1:A:442:GLN:HE21	1:A:442:GLN:HA	1.84	0.42
1:B:290:ASN:ND2	1:B:292:ASP:H	2.17	0.42
1:A:417:HIS:HD2	1:A:421:ILE:HD11	1.83	0.42
1:A:555:PHE:HA	1:A:558:LEU:HB2	2.02	0.42
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.95	0.42
1:B:248:LEU:HD21	1:B:278:LEU:HD22	2.02	0.42
1:B:305:GLN:O	1:B:309:LYS:HB2	2.20	0.42
1:B:407:ILE:HD13	1:B:407:ILE:HA	1.76	0.42
2:E:372:THR:HG22	2:E:374:LEU:HD12	2.02	0.41
1:A:491:VAL:HG13	1:A:492:PRO:HD2	2.01	0.41
1:A:349:TRP:HB3	1:A:351:LEU:HD12	2.02	0.41
1:A:505:HIS:CD2	1:A:505:HIS:H	2.38	0.41
1:B:229:THR:HG23	1:B:516:TYR:OH	2.19	0.41
1:A:514:ARG:HG2	1:A:515:TYR:N	2.35	0.41
2:E:329:PHE:CD2	2:E:329:PHE:N	2.83	0.41
2:F:369:VAL:O	2:F:370:SER:HB2	2.20	0.41
1:A:85:LEU:HD23	1:A:85:LEU:N	2.32	0.41
2:E:404:VAL:H	2:E:407:ASP:CB	2.31	0.41
1:A:320:LEU:HD13	1:A:380:GLN:HG2	2.02	0.41
1:B:239:HIS:O	1:B:240:LEU:C	2.58	0.41
1:B:412:ALA:HA	1:B:417:HIS:CD2	2.56	0.41
1:B:489:GLU:HG2	1:B:613:TYR:HE2	1.86	0.41
2:F:404:VAL:N	2:F:407:ASP:HB2	2.34	0.41
1:B:212:VAL:HB	1:B:215:TYR:HB2	2.03	0.41
2:F:422:ALA:HB2	2:F:496:VAL:HG22	2.01	0.41
1:A:560:LEU:O	1:A:563:SER:HB2	2.21	0.41
2:E:408:TYR:CD2	2:E:444:ARG:HB3	2.56	0.41
1:A:489:GLU:HG2	1:A:489:GLU:O	2.21	0.40
1:A:212:VAL:O	1:A:213:ASP:HB2	2.20	0.40
1:B:54:ILE:HG13	1:B:341:LYS:O	2.22	0.40
1:B:85:LEU:H	1:B:85:LEU:HD23	1.86	0.40
1:B:167:SER:O	1:B:171:GLU:HG2	2.21	0.40
1:A:454:TYR:OH	1:A:458:LYS:HD3	2.22	0.40
2:F:472:LEU:O	2:F:473:ASN:HB2	2.21	0.40
1:A:493:HIS:CD2	1:A:499:ASP:OD1	2.61	0.40
1:B:388:GLN:OE1	1:B:389:PRO:HD2	2.22	0.40
2:E:339:ALA:HA	2:E:455:ILE:HD11	2.03	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%)	540 (91%)	51 (9%)	4 (1%)	22 53
1	B	595/597 (100%)	546 (92%)	40 (7%)	9 (2%)	10 33
2	E	169/179 (94%)	138 (82%)	23 (14%)	8 (5%)	2 7
2	F	169/179 (94%)	141 (83%)	22 (13%)	6 (4%)	3 11
All	All	1528/1552 (98%)	1365 (89%)	136 (9%)	27 (2%)	8 28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	VAL
2	E	404	VAL
2	F	369	VAL
2	F	370	SER
1	B	536	GLU
2	E	416	PHE
2	F	368	GLY
2	F	416	PHE
1	B	20	THR
1	B	87	GLU
1	B	212	VAL
1	B	213	ASP
2	E	358	SER
2	E	368	GLY
2	F	465	LYS
1	B	340	GLN
2	E	330	ASN
2	E	402	THR
2	E	465	LYS
1	A	289	PRO
1	A	339	VAL
2	E	401	GLN

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Mol	Chain	Res	Type
1	B	84	PRO
1	B	339	VAL
1	B	54	ILE
1	A	147	GLY
2	F	391	GLY

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%)	474 (90%)	53 (10%)	7 22
1	B	527/527 (100%)	473 (90%)	54 (10%)	7 22
2	E	151/157 (96%)	129 (85%)	22 (15%)	3 9
2	F	151/157 (96%)	129 (85%)	22 (15%)	3 9
All	All	1356/1368 (99%)	1205 (89%)	151 (11%)	6 19

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	29	LEU
1	A	55	THR
1	A	60	GLN
1	A	78	THR
1	A	81	GLN
1	A	85	LEU
1	A	86	GLN
1	A	90	ASN
1	A	100	LEU
1	A	103	ASN
1	A	114	LYS
1	A	129	THR
1	A	148	LEU
1	A	156	LEU
1	A	198	ASP

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	240	LEU
1	A	283	VAL
1	A	292	ASP
1	A	293	VAL
1	A	334	THR
1	A	343	VAL
1	A	364	VAL
1	A	368	ASP
1	A	371	THR
1	A	375	GLU
1	A	381	TYR
1	A	385	TYR
1	A	392	LEU
1	A	401	HIS
1	A	410	LEU
1	A	418	LEU
1	A	439	LEU
1	A	444	LEU
1	A	449	THR
1	A	455	MET
1	A	456	LEU
1	A	460	ARG
1	A	476	LYS
1	A	488	VAL
1	A	503	LEU
1	A	514	ARG
1	A	518	ARG
1	A	526	GLN
1	A	549	GLU
1	A	557	MET
1	A	562	LYS
1	A	573	VAL
1	A	585	LEU
1	A	595	LEU
1	A	597	ASP
1	A	600	LYS
1	B	29	LEU
1	B	81	GLN
1	B	89	GLN
1	B	98	GLN
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	103	ASN
1	B	114	LYS
1	B	121	ASN
1	B	125	THR
1	B	137	ASN
1	B	148	LEU
1	B	156	LEU
1	B	187	LYS
1	B	198	ASP
1	B	212	VAL
1	B	240	LEU
1	B	271	TRP
1	B	290	ASN
1	B	291	ILE
1	B	309	LYS
1	B	313	LYS
1	B	333	LEU
1	B	334	THR
1	B	343	VAL
1	B	357	ARG
1	B	360	MET
1	B	375	GLU
1	B	381	TYR
1	B	385	TYR
1	B	392	LEU
1	B	401	HIS
1	B	410	LEU
1	B	416	LYS
1	B	418	LEU
1	B	421	ILE
1	B	427	ASP
1	B	429	GLN
1	B	432	ASN
1	B	439	LEU
1	B	444	LEU
1	B	455	MET
1	B	456	LEU
1	B	488	VAL
1	B	493	HIS
1	B	496	THR
1	B	503	LEU
1	B	526	GLN

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Mol	Chain	Res	Type
1	B	529	LEU
1	B	549	GLU
1	B	553	LYS
1	B	557	MET
1	B	560	LEU
1	B	585	LEU
1	B	593	THR
2	E	329	PHE
2	E	332	THR
2	E	333	LYS
2	E	337	VAL
2	E	338	TYR
2	E	364	PHE
2	E	369	VAL
2	E	395	ARG
2	E	412	LEU
2	E	415	ASP
2	E	416	PHE
2	E	417	MET
2	E	423	TRP
2	E	433	THR
2	E	447	LYS
2	E	455	ILE
2	E	467	CYS
2	E	468	THR
2	E	472	LEU
2	E	480	ASP
2	E	481	TYR
2	E	484	TYR
2	F	329	PHE
2	F	333	LYS
2	F	337	VAL
2	F	341	GLU
2	F	344	LYS
2	F	359	THR
2	F	360	PHE
2	F	364	PHE
2	F	369	VAL
2	F	372	THR
2	F	373	LYS
2	F	390	LYS
2	F	395	ARG

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Mol	Chain	Res	Type
2	F	399	PRO
2	F	412	LEU
2	F	415	ASP
2	F	416	PHE
2	F	417	MET
2	F	426	ARG
2	F	427	ASN
2	F	455	ILE
2	F	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	51	ASN
1	A	60	GLN
1	A	64	ASN
1	A	90	ASN
1	A	101	GLN
1	A	103	ASN
1	A	137	ASN
1	A	149	ASN
1	A	221	GLN
1	A	325	GLN
1	A	442	GLN
1	A	493	HIS
1	A	505	HIS
1	A	524	GLN
1	A	526	GLN
1	A	546	ASN
1	A	586	ASN
1	A	599	ASN
1	B	33	ASN
1	B	51	ASN
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	429	GLN

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Mol	Chain	Res	Type
1	B	493	HIS
1	B	505	HIS
1	B	524	GLN
1	B	526	GLN
1	B	546	ASN
1	B	586	ASN
1	B	599	ASN
1	B	601	ASN
2	F	375	ASN
2	F	409	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	618	-	15,15,15	0.57	0	21,21,21	2.14	3 (14%)
3	NDG	B	617	-	15,15,15	0.78	0	21,21,21	1.48	3 (14%)
3	NDG	A	616	-	15,15,15	0.48	0	21,21,21	1.22	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NDG	B	616	-	15,15,15	0.42	0	21,21,21	0.73	0
6	NAG	E	91	-	15,15,15	0.55	0	21,21,21	1.63	4 (19%)
3	NDG	F	91	-	15,15,15	0.49	0	21,21,21	1.08	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	-	-	2/6/26/26	0/1/1/1
3	NDG	B	617	-	-	4/6/26/26	0/1/1/1
3	NDG	A	616	-	-	6/6/26/26	0/1/1/1
3	NDG	B	616	-	-	4/6/26/26	0/1/1/1
6	NAG	E	91	-	-	4/6/26/26	0/1/1/1
3	NDG	F	91	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	618	NDG	O5-C1-C2	7.95	117.51	109.52
3	B	617	NDG	O5-C1-C2	4.39	113.93	109.52
6	E	91	NAG	O5-C1-C2	3.68	113.22	109.52
6	E	91	NAG	C1-O5-C5	3.37	120.17	113.65
3	F	91	NDG	O5-C1-C2	2.98	112.52	109.52
3	B	618	NDG	C1-O5-C5	2.81	119.09	113.65
3	A	616	NDG	C4-C3-C2	2.74	114.39	110.40
3	B	618	NDG	C1-C2-C3	2.46	113.90	110.54
6	E	91	NAG	C1-C2-C3	2.38	113.78	110.54
6	E	91	NAG	O5-C5-C4	2.34	113.91	109.70
3	B	617	NDG	C3-C2-N2	2.27	114.80	110.62
3	B	617	NDG	O7-C7-C8	-2.16	118.22	122.05
3	F	91	NDG	C4-C3-C2	2.14	113.53	110.40
3	A	616	NDG	C3-C4-C5	2.14	114.12	110.23
3	A	616	NDG	C1-C2-C3	2.06	113.35	110.54

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
6	E	91	NAG	C8-C7-N2-C2
6	E	91	NAG	O7-C7-N2-C2
3	B	616	NDG	O5-C5-C6-O6
3	A	616	NDG	O5-C5-C6-O6
3	B	617	NDG	O5-C5-C6-O6
3	B	616	NDG	C4-C5-C6-O6
3	B	618	NDG	O5-C5-C6-O6
3	A	616	NDG	C4-C5-C6-O6
3	B	618	NDG	C4-C5-C6-O6
3	B	617	NDG	C4-C5-C6-O6
3	A	616	NDG	C3-C2-N2-C7
6	E	91	NAG	C4-C5-C6-O6
3	F	91	NDG	C8-C7-N2-C2
3	F	91	NDG	O7-C7-N2-C2
3	A	616	NDG	C1-C2-N2-C7
6	E	91	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	618	NDG	3	0
3	B	617	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%)	0.38	40 (6%)	17	10	41, 69, 119, 141	0
1	B	597/597 (100%)	0.34	32 (5%)	25	17	37, 65, 119, 139	0
2	E	173/179 (96%)	0.67	24 (13%)	2	1	54, 79, 123, 135	0
2	F	173/179 (96%)	0.39	7 (4%)	38	28	55, 80, 122, 134	0
All	All	1540/1552 (99%)	0.40	103 (6%)	17	10	37, 70, 121, 141	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	SER	7.9
1	A	339	VAL	7.4
1	B	86	GLN	6.6
1	A	290	ASN	5.9
2	E	501	PHE	5.8
1	A	104	GLY	5.0
1	B	89	GLN	4.7
1	A	425	SER	4.7
1	B	615	ASP	4.6
1	A	108	LEU	4.5
2	E	353	SER	4.3
1	A	338	ASN	4.2
2	E	356	TYR	4.2
1	B	140	GLU	4.1
1	B	339	VAL	4.0
1	A	428	PHE	3.9
1	A	107	VAL	3.8
1	B	139	GLN	3.8
1	B	136	ASP	3.7
1	A	106	SER	3.7
2	E	369	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	500	SER	3.7
1	A	54	ILE	3.5
1	B	137	ASN	3.4
1	A	89	GLN	3.4
1	B	97	LEU	3.4
1	A	192	ARG	3.3
2	E	352	TYR	3.3
1	B	83	TYR	3.2
1	A	19	SER	3.2
2	F	358	SER	3.2
1	B	338	ASN	3.2
2	E	472	LEU	3.1
1	A	342	ALA	3.1
1	A	291	ILE	3.1
1	A	364	VAL	3.1
1	A	196	TYR	3.1
2	E	359	THR	3.1
1	A	424	LEU	3.0
1	A	292	ASP	3.0
1	A	81	GLN	3.0
2	E	357	ASN	2.9
1	B	105	SER	2.9
1	B	60	GLN	2.9
1	A	60	GLN	2.9
1	B	106	SER	2.9
1	A	297	MET	2.9
2	E	402	THR	2.8
2	E	354	VAL	2.8
1	A	363	LYS	2.8
1	B	85	LEU	2.7
2	F	419	CYS	2.7
1	A	55	THR	2.7
1	A	427	ASP	2.6
1	B	92	THR	2.6
2	E	421	LEU	2.6
1	B	141	CYS	2.5
1	B	213	ASP	2.5
1	B	214	GLY	2.5
2	E	364	PHE	2.5
1	A	336	PRO	2.5
1	B	88	ILE	2.5
1	A	301	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	19	SER	2.5
2	F	356	TYR	2.5
1	A	91	LEU	2.5
2	F	350	ALA	2.5
1	B	367	ASP	2.5
1	A	344	CYS	2.4
1	B	429	GLN	2.4
1	B	134	ASN	2.4
1	A	337	GLY	2.4
1	B	21	THR	2.4
2	E	351	ASP	2.4
1	A	132	VAL	2.3
2	E	349	VAL	2.3
2	F	354	VAL	2.3
2	E	419	CYS	2.3
2	E	345	ILE	2.3
1	A	302	TRP	2.3
1	B	294	THR	2.3
2	E	355	LEU	2.3
1	A	299	ASP	2.3
2	E	415	ASP	2.3
2	F	472	LEU	2.2
2	E	325	PHE	2.2
2	E	383	TYR	2.2
1	B	94	LYS	2.2
2	E	350	ALA	2.2
2	E	428	ILE	2.2
1	B	69	TRP	2.2
1	A	103	ASN	2.2
1	A	340	GLN	2.2
1	B	100	LEU	2.1
1	B	54	ILE	2.1
1	A	56	GLU	2.1
1	A	214	GLY	2.1
1	B	290	ASN	2.1
1	A	361	CYS	2.1
2	E	382	VAL	2.1
2	F	445	HIS	2.0
1	B	572	ASN	2.0
1	A	298	VAL	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	0.56	0.32	127,128,129,129	0
3	NDG	B	617	15/15	0.66	0.23	79,88,90,90	0
3	NDG	F	91	15/15	0.76	0.23	118,119,119,120	0
3	NDG	B	618	15/15	0.79	0.19	68,71,76,77	0
3	NDG	B	616	15/15	0.80	0.30	97,97,98,98	0
4	ZN	A	901	1/1	0.89	0.21	85,85,85,85	0
3	NDG	A	616	15/15	0.89	0.25	109,109,110,111	0
5	CL	A	902	1/1	0.95	0.27	66,66,66,66	0
4	ZN	B	901	1/1	0.97	0.26	81,81,81,81	0
5	CL	B	902	1/1	0.99	0.16	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.