Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 09:40 PM EDT

PDB ID	:	1N04
Title	:	Diferric chicken serum transferrin at 2.8 A resolution.
Authors	:	Guha Thakurta, P.; Choudhury, D.; Dasgupta, R.; Dattagupta, J.K.
Deposited on	:	2002-10-11
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:

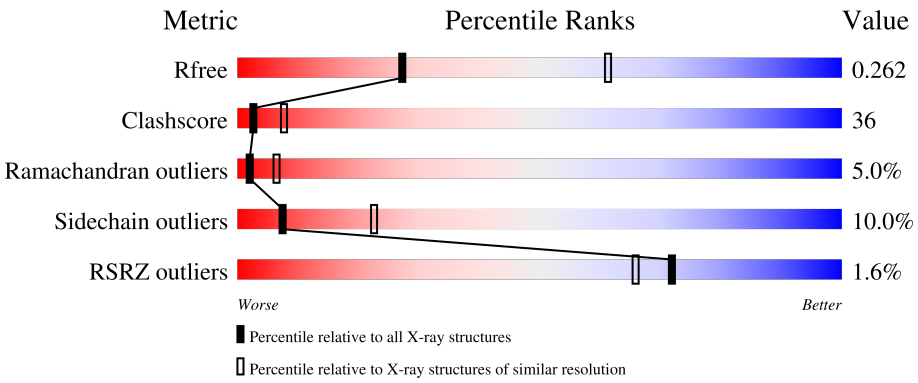
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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))
R_{free}	130704	3140 (2.80-2.80)
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	686	2% 51% 40% 8% •

2 Entry composition (i)

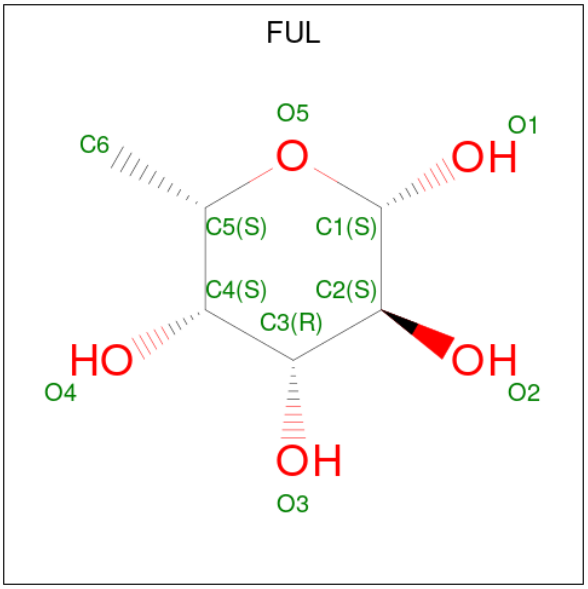
There are 5 unique types of molecules in this entry. The entry contains 5307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 serum transferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	683	5232	3270	909	1012	41	0	0	0

- Molecule 2 is beta-L-fucopyranose (three-letter code: FUL) (formula: $C_6H_{12}O_5$).

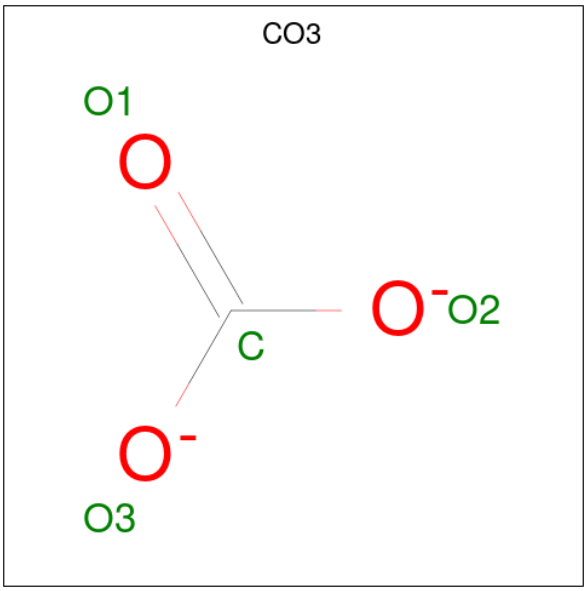


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	11	6	5	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	A	2	2	2	0	0

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 5 is water.

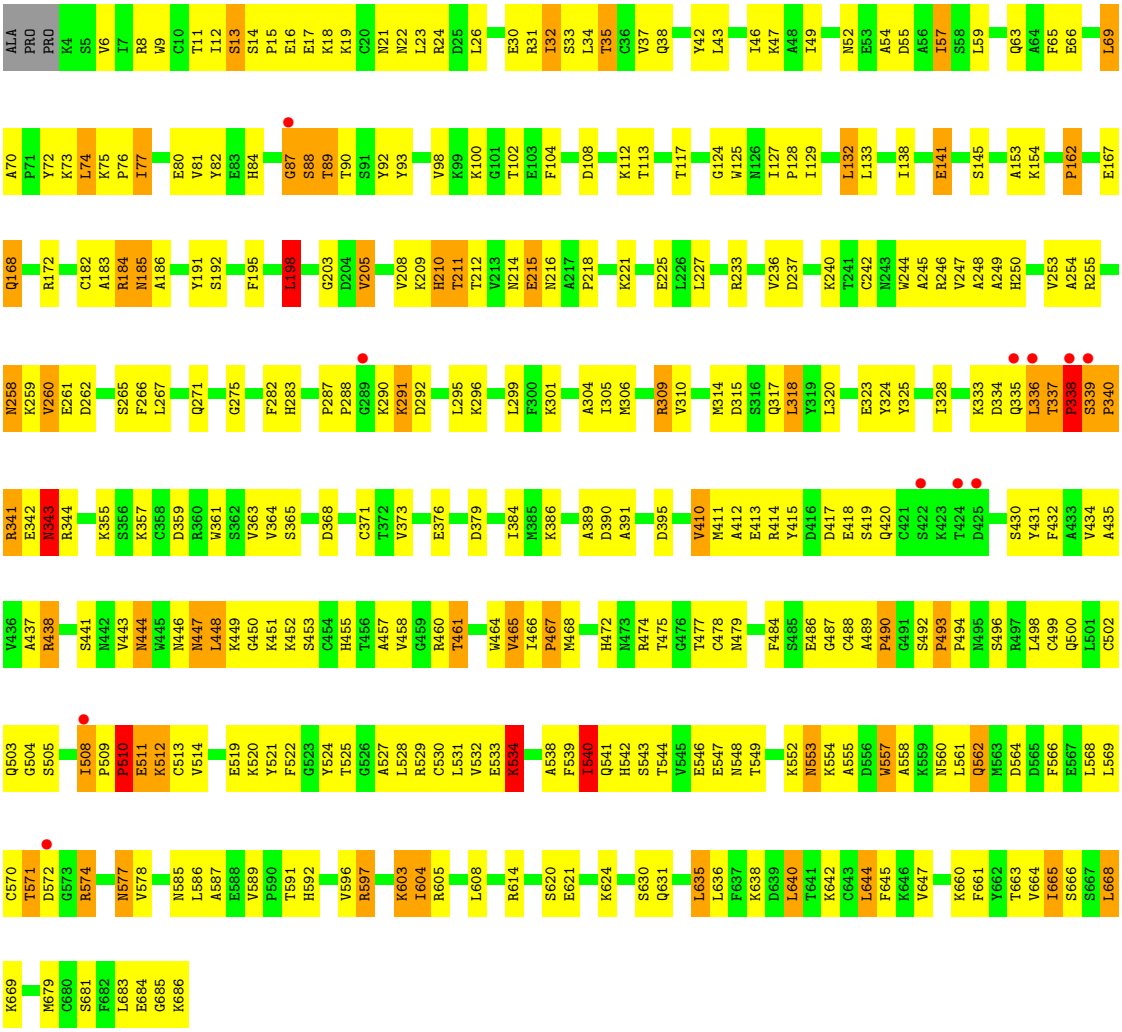
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	54	54	54	0	0

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: serum transferrin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.96Å 59.11Å 81.86Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	14.97 – 2.80 14.97 – 2.76	Depositor EDS
% Data completeness (in resolution range)	91.1 (14.97-2.80) 88.1 (14.97-2.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.269 0.211 , 0.262	Depositor DCC
R_{free} test set	768 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.4	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	5307	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: FUL, FE, CO3

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	0.39	0/5336	0.68	1/7213 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	LEU	CA-CB-CG	5.29	127.48	115.30

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	5232	0	5039	376	0
2	A	11	0	12	4	0
3	A	2	0	0	0	0
4	A	8	0	0	1	0
5	A	54	0	0	4	0
All	All	5307	0	5051	376	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 36.

All (376) 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:A:16:GLU:HG2	1:A:299:LEU:HD22	1.27	1.09
1:A:6:VAL:HG12	1:A:33:SER:HB3	1.27	1.09
1:A:525:THR:HG22	1:A:548:ASN:HD21	1.16	1.07
1:A:335:GLN:O	1:A:338:PRO:HD2	1.59	1.02
1:A:504:GLY:HA2	1:A:512:LYS:HA	1.42	1.00
1:A:597:ARG:HH11	1:A:597:ARG:HB3	1.24	0.98
1:A:258:ASN:HD22	1:A:258:ASN:N	1.65	0.94
1:A:508:ILE:HB	1:A:509:PRO:HD3	1.50	0.93
1:A:218:PRO:HD2	1:A:290:LYS:HE2	1.51	0.93
1:A:553:ASN:HD22	1:A:554:LYS:N	1.68	0.91
1:A:444:ASN:HD22	1:A:447:ASN:HB2	1.37	0.90
1:A:534:LYS:HA	1:A:534:LYS:HE2	1.54	0.90
1:A:32:ILE:H	1:A:32:ILE:HD12	1.38	0.88
1:A:488:CYS:HA	1:A:498:LEU:O	1.76	0.85
1:A:335:GLN:O	1:A:337:THR:N	2.13	0.82
1:A:508:ILE:HB	1:A:509:PRO:CD	2.10	0.81
1:A:291:LYS:HE3	1:A:296:LYS:HG2	1.60	0.81
1:A:355:LYS:HZ3	1:A:371:CYS:HB2	1.45	0.81
1:A:592:HIS:CE1	1:A:638:LYS:HD3	2.16	0.80
1:A:418:GLU:HA	1:A:642:LYS:HB3	1.63	0.78
1:A:434:VAL:HG11	1:A:568:LEU:HD22	1.66	0.77
1:A:209:LYS:NZ	1:A:301:LYS:HZ3	1.83	0.77
1:A:258:ASN:HD22	1:A:258:ASN:H	1.28	0.77
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.49	0.76
1:A:531:LEU:HB2	1:A:538:ALA:HB2	1.67	0.76
1:A:443:VAL:HG22	1:A:451:LYS:HZ3	1.50	0.76
1:A:318:LEU:HD13	1:A:386:LYS:HE2	1.67	0.75
1:A:365:SER:HA	1:A:614:ARG:NH2	2.01	0.75
1:A:505:SER:HB2	1:A:511:GLU:HB2	1.68	0.75
1:A:597:ARG:HB3	1:A:597:ARG:NH1	2.01	0.75
1:A:104:PHE:HB2	1:A:108:ASP:HB2	1.69	0.74
1:A:414:ARG:HD3	1:A:420:GLN:HB2	1.68	0.74
1:A:49:ILE:O	1:A:255:ARG:HD3	1.87	0.73
1:A:153:ALA:CB	1:A:167:GLU:HG2	2.19	0.73
1:A:343:ASN:CG	1:A:603:LYS:HZ1	1.91	0.73
1:A:214:ASN:O	1:A:218:PRO:HG3	1.88	0.72
1:A:577:ASN:HD22	1:A:578:VAL:N	1.88	0.72
1:A:113:THR:OG1	1:A:203:GLY:HA2	1.90	0.72
1:A:162:PRO:HB3	1:A:183:ALA:O	1.90	0.72
1:A:16:GLU:HG2	1:A:299:LEU:CD2	2.13	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:PHE:CE2	1:A:665:ILE:HD11	2.25	0.71
1:A:458:VAL:HG21	1:A:492:SER:OG	1.90	0.71
1:A:630:SER:HB2	1:A:635:LEU:HD22	1.73	0.71
1:A:52:ASN:ND2	2:A:691:FUL:H1	2.04	0.71
1:A:413:GLU:HA	1:A:644:LEU:HD12	1.72	0.71
1:A:141:GLU:HG3	1:A:145:SER:HB3	1.73	0.70
1:A:444:ASN:ND2	1:A:447:ASN:HB2	2.05	0.70
1:A:525:THR:CG2	1:A:548:ASN:HD21	2.00	0.69
1:A:338:PRO:O	1:A:340:PRO:HD2	1.93	0.69
1:A:508:ILE:CB	1:A:509:PRO:HD3	2.22	0.69
1:A:621:GLU:OE1	1:A:624:LYS:HD2	1.93	0.69
1:A:410:VAL:HG13	1:A:411:MET:HG2	1.76	0.68
1:A:435:ALA:HB3	1:A:569:LEU:HB2	1.74	0.68
1:A:527:ALA:HB3	1:A:540:ILE:CD1	2.23	0.68
1:A:664:VAL:O	1:A:668:LEU:HB2	1.94	0.68
1:A:596:VAL:HG11	1:A:604:ILE:CD1	2.24	0.68
1:A:141:GLU:CG	1:A:145:SER:HB3	2.24	0.67
1:A:258:ASN:N	1:A:258:ASN:ND2	2.40	0.67
1:A:546:GLU:O	1:A:546:GLU:HG3	1.94	0.67
1:A:185:ASN:HD22	1:A:185:ASN:H	1.42	0.67
1:A:540:ILE:HG23	1:A:541:GLN:N	2.08	0.67
1:A:683:LEU:O	1:A:685:GLY:N	2.27	0.67
1:A:32:ILE:H	1:A:32:ILE:CD1	2.03	0.67
1:A:553:ASN:HD22	1:A:553:ASN:C	1.97	0.67
1:A:84:HIS:HB2	1:A:88:SER:HA	1.76	0.66
1:A:417:ASP:HB3	1:A:420:GLN:CG	2.26	0.66
1:A:577:ASN:HD22	1:A:578:VAL:H	1.41	0.66
1:A:452:LYS:HA	1:A:486:GLU:O	1.95	0.66
1:A:77:ILE:HD13	1:A:254:ALA:HB3	1.77	0.66
1:A:117:THR:OG1	1:A:124:GLY:HA3	1.95	0.66
1:A:417:ASP:HB3	1:A:420:GLN:HG2	1.78	0.66
1:A:66:GLU:HA	1:A:69:LEU:HD22	1.78	0.66
1:A:258:ASN:H	1:A:258:ASN:ND2	1.94	0.66
1:A:475:THR:HG22	1:A:477:THR:OG1	1.95	0.66
1:A:47:LYS:HE2	1:A:72:TYR:OH	1.95	0.66
1:A:524:TYR:O	1:A:540:ILE:HD11	1.96	0.66
1:A:12:ILE:O	1:A:13:SER:HB3	1.96	0.66
1:A:209:LYS:NZ	1:A:301:LYS:NZ	2.45	0.65
1:A:209:LYS:HZ3	1:A:301:LYS:HZ3	1.44	0.65
1:A:434:VAL:CG1	1:A:568:LEU:HD22	2.26	0.65
1:A:291:LYS:HG2	1:A:292:ASP:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:O	1:A:90:THR:HG22	1.96	0.64
1:A:490:PRO:HG2	1:A:522:PHE:HA	1.80	0.64
1:A:525:THR:HG22	1:A:548:ASN:ND2	2.01	0.64
1:A:521:TYR:CG	1:A:530:CYS:HB2	2.33	0.64
1:A:541:GLN:OE1	1:A:640:LEU:HD12	1.98	0.63
1:A:509:PRO:O	1:A:510:PRO:C	2.36	0.63
1:A:291:LYS:CE	1:A:296:LYS:HG2	2.28	0.63
1:A:504:GLY:HA2	1:A:512:LYS:CA	2.23	0.63
1:A:30:GLU:OE1	1:A:30:GLU:HA	1.99	0.63
1:A:477:THR:HG22	1:A:478:CYS:N	2.14	0.62
1:A:410:VAL:HG22	1:A:605:ARG:NE	2.14	0.62
1:A:247:VAL:HG12	1:A:248:ALA:H	1.65	0.62
1:A:98:VAL:HG12	1:A:205:VAL:HG13	1.82	0.62
1:A:65:PHE:O	1:A:69:LEU:HD13	1.99	0.61
1:A:447:ASN:HB3	1:A:451:LYS:NZ	2.15	0.61
1:A:339:SER:CB	1:A:340:PRO:HD3	2.31	0.61
1:A:215:GLU:HB2	5:A:696:HOH:O	2.00	0.61
1:A:415:TYR:HB3	1:A:640:LEU:HD13	1.82	0.61
1:A:533:GLU:O	1:A:533:GLU:HG3	1.99	0.61
1:A:355:LYS:NZ	1:A:359:ASP:OD1	2.23	0.61
1:A:410:VAL:HG22	1:A:605:ARG:CZ	2.31	0.61
1:A:34:LEU:HB2	1:A:266:PHE:CE2	2.36	0.60
1:A:549:THR:O	1:A:552:LYS:HE2	2.01	0.60
1:A:52:ASN:ND2	2:A:691:FUL:C1	2.64	0.60
1:A:418:GLU:CA	1:A:642:LYS:HB3	2.31	0.60
1:A:23:LEU:HD13	1:A:282:PHE:HE2	1.67	0.60
1:A:315:ASP:OD2	1:A:318:LEU:HB2	2.01	0.60
1:A:510:PRO:O	1:A:511:GLU:HB2	2.01	0.60
1:A:24:ARG:HG2	1:A:24:ARG:NH1	2.16	0.60
1:A:508:ILE:CB	1:A:509:PRO:CD	2.78	0.60
1:A:549:THR:HG22	1:A:561:LEU:HB3	1.84	0.60
1:A:464:TRP:C	1:A:467:PRO:HD2	2.21	0.60
1:A:665:ILE:O	1:A:669:LYS:HB2	2.02	0.59
1:A:98:VAL:HG11	1:A:227:LEU:HD22	1.85	0.59
1:A:324:TYR:CE2	1:A:328:ILE:HD11	2.37	0.59
1:A:324:TYR:CZ	1:A:328:ILE:HD11	2.38	0.59
1:A:339:SER:CB	1:A:340:PRO:CD	2.81	0.59
1:A:11:THR:OG1	1:A:38:GLN:HA	2.03	0.59
1:A:250:HIS:CE1	1:A:301:LYS:HD2	2.38	0.58
1:A:630:SER:O	1:A:631:GLN:HB2	2.03	0.58
1:A:338:PRO:O	1:A:340:PRO:CD	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HD3	1:A:373:VAL:HB	1.85	0.58
1:A:414:ARG:CD	1:A:420:GLN:HB2	2.33	0.58
1:A:108:ASP:O	1:A:112:LYS:HE3	2.02	0.58
1:A:77:ILE:HG21	1:A:260:VAL:HG13	1.85	0.58
1:A:499:CYS:O	1:A:502:CYS:HB2	2.03	0.58
1:A:570:CYS:O	1:A:572:ASP:N	2.37	0.58
1:A:208:VAL:HB	1:A:212:THR:OG1	2.04	0.58
1:A:184:ARG:HG3	1:A:184:ARG:HH11	1.68	0.57
1:A:185:ASN:H	1:A:185:ASN:ND2	2.01	0.57
1:A:340:PRO:O	1:A:341:ARG:CB	2.52	0.57
1:A:290:LYS:O	1:A:291:LYS:HB2	2.03	0.57
1:A:568:LEU:HG	1:A:578:VAL:HA	1.87	0.57
1:A:23:LEU:HD13	1:A:282:PHE:CE2	2.40	0.57
1:A:489:ALA:O	1:A:492:SER:HB2	2.04	0.57
1:A:8:ARG:O	1:A:55:ASP:HB2	2.05	0.57
1:A:539:PHE:O	1:A:540:ILE:HD12	2.05	0.56
1:A:185:ASN:ND2	1:A:185:ASN:N	2.52	0.56
1:A:553:ASN:ND2	1:A:555:ALA:H	2.03	0.56
1:A:533:GLU:O	1:A:534:LYS:HB2	2.04	0.56
1:A:447:ASN:C	1:A:449:LYS:H	2.09	0.56
1:A:604:ILE:O	1:A:608:LEU:HB2	2.06	0.56
1:A:457:ALA:HB3	1:A:460:ARG:CD	2.36	0.56
1:A:503:GLN:HG2	1:A:521:TYR:CE2	2.40	0.55
1:A:533:GLU:O	1:A:534:LYS:CB	2.54	0.55
1:A:361:TRP:HA	1:A:364:VAL:HG12	1.87	0.55
1:A:532:VAL:HG22	1:A:566:PHE:HZ	1.71	0.55
1:A:534:LYS:HA	1:A:534:LYS:CE	2.33	0.55
1:A:22:ASN:O	1:A:26:LEU:HD13	2.05	0.55
1:A:19:LYS:HD2	1:A:299:LEU:HD23	1.88	0.55
1:A:98:VAL:CG1	1:A:205:VAL:HG13	2.35	0.55
1:A:337:THR:O	1:A:338:PRO:C	2.45	0.55
1:A:438:ARG:HB2	1:A:441:SER:HB2	1.89	0.55
1:A:596:VAL:HG11	1:A:604:ILE:HD13	1.88	0.55
1:A:52:ASN:HD22	2:A:691:FUL:H1	1.70	0.55
1:A:338:PRO:O	1:A:340:PRO:N	2.40	0.55
1:A:574:ARG:H	1:A:574:ARG:CD	2.20	0.54
1:A:98:VAL:CG1	1:A:227:LEU:HD22	2.36	0.54
1:A:250:HIS:CD2	1:A:301:LYS:HD2	2.43	0.54
1:A:283:HIS:CG	1:A:287:PRO:HD3	2.43	0.54
1:A:291:LYS:HG2	1:A:292:ASP:H	1.72	0.54
1:A:314:MET:HG2	1:A:679:MET:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HA	1:A:389:ALA:O	2.07	0.54
1:A:52:ASN:ND2	2:A:691:FUL:O1	2.40	0.54
1:A:504:GLY:O	1:A:519:GLU:HA	2.07	0.54
1:A:477:THR:HG22	1:A:479:ASN:H	1.72	0.54
1:A:208:VAL:HG11	1:A:212:THR:HG21	1.89	0.54
1:A:209:LYS:HZ2	1:A:301:LYS:NZ	2.04	0.54
1:A:457:ALA:HB3	1:A:460:ARG:HD3	1.90	0.54
1:A:432:PHE:H	1:A:542:HIS:HD2	1.55	0.54
1:A:466:ILE:HB	1:A:467:PRO:HD3	1.90	0.54
1:A:534:LYS:HE2	1:A:534:LYS:CA	2.33	0.54
1:A:271:GLN:O	1:A:275:GLY:N	2.41	0.53
1:A:447:ASN:HB3	1:A:451:LYS:HZ2	1.73	0.53
1:A:455:HIS:HB2	1:A:489:ALA:HB2	1.89	0.53
1:A:19:LYS:HB3	1:A:299:LEU:CD2	2.39	0.53
1:A:125:TRP:C	1:A:128:PRO:HD2	2.28	0.53
1:A:511:GLU:O	1:A:514:VAL:HG12	2.08	0.53
1:A:412:ALA:HB3	1:A:645:PHE:CE2	2.44	0.53
1:A:493:PRO:HB2	1:A:496:SER:HB3	1.91	0.53
1:A:527:ALA:HB3	1:A:540:ILE:HD11	1.91	0.53
1:A:540:ILE:HG21	1:A:544:THR:HB	1.90	0.53
1:A:185:ASN:HD22	1:A:185:ASN:N	2.02	0.53
1:A:192:SER:OG	1:A:296:LYS:HD2	2.09	0.53
1:A:490:PRO:HB3	1:A:514:VAL:O	2.09	0.53
1:A:9:TRP:CZ3	1:A:267:LEU:HD21	2.44	0.52
1:A:247:VAL:HG12	1:A:248:ALA:N	2.24	0.52
1:A:570:CYS:O	1:A:571:THR:C	2.48	0.52
1:A:65:PHE:HB2	1:A:320:LEU:HD11	1.89	0.52
1:A:447:ASN:O	1:A:449:LYS:N	2.43	0.52
1:A:77:ILE:CD1	1:A:254:ALA:HB3	2.39	0.52
1:A:80:GLU:OE2	1:A:304:ALA:HB2	2.10	0.52
1:A:259:LYS:O	1:A:262:ASP:N	2.41	0.52
1:A:292:ASP:HB3	1:A:295:LEU:HG	1.92	0.52
1:A:415:TYR:HE2	1:A:431:TYR:CD1	2.28	0.52
1:A:455:HIS:HB2	1:A:489:ALA:CB	2.39	0.52
1:A:524:TYR:HD1	1:A:540:ILE:HG13	1.75	0.52
1:A:543:SER:O	1:A:547:GLU:HG3	2.10	0.52
1:A:681:SER:O	1:A:685:GLY:O	2.28	0.52
1:A:395:ASP:HA	1:A:592:HIS:CD2	2.45	0.52
1:A:553:ASN:C	1:A:553:ASN:ND2	2.64	0.51
1:A:540:ILE:HG23	1:A:541:GLN:O	2.10	0.51
1:A:577:ASN:ND2	1:A:578:VAL:N	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:OG	1:A:16:GLU:HB2	2.10	0.51
1:A:57:ILE:HG23	1:A:59:LEU:HD21	1.93	0.51
1:A:240:LYS:HE3	5:A:701:HOH:O	2.10	0.51
1:A:343:ASN:CG	1:A:603:LYS:NZ	2.64	0.51
1:A:250:HIS:CG	1:A:301:LYS:HD2	2.45	0.51
1:A:70:ALA:HB2	1:A:73:LYS:HE2	1.92	0.51
1:A:72:TYR:HB3	1:A:74:LEU:HD22	1.93	0.51
1:A:431:TYR:HE1	1:A:591:THR:HA	1.76	0.50
1:A:259:LYS:O	1:A:260:VAL:C	2.49	0.50
1:A:19:LYS:HB3	1:A:299:LEU:HD23	1.92	0.50
1:A:444:ASN:ND2	1:A:447:ASN:N	2.59	0.50
1:A:191:TYR:CE2	1:A:301:LYS:HE3	2.46	0.50
1:A:6:VAL:HG12	1:A:33:SER:CB	2.19	0.50
1:A:43:LEU:O	1:A:47:LYS:HG3	2.11	0.49
1:A:283:HIS:CD2	1:A:287:PRO:HD3	2.47	0.49
1:A:153:ALA:HB3	1:A:167:GLU:HG2	1.93	0.49
1:A:183:ALA:H	1:A:186:ALA:HB2	1.77	0.49
1:A:81:VAL:O	1:A:305:ILE:HG12	2.12	0.49
1:A:417:ASP:HB3	1:A:420:GLN:HG3	1.94	0.49
1:A:34:LEU:HD13	1:A:266:PHE:CZ	2.48	0.49
1:A:133:LEU:HD23	1:A:138:ILE:HB	1.94	0.49
1:A:477:THR:HG22	1:A:478:CYS:H	1.74	0.49
1:A:14:SER:N	1:A:15:PRO:CD	2.75	0.49
1:A:132:LEU:HB3	1:A:138:ILE:HG13	1.95	0.49
1:A:127:ILE:HB	1:A:128:PRO:HD3	1.93	0.49
1:A:342:GLU:O	1:A:343:ASN:OD1	2.31	0.49
1:A:16:GLU:CG	1:A:299:LEU:HD22	2.20	0.49
1:A:100:LYS:HA	1:A:225:GLU:OE1	2.13	0.49
1:A:357:LYS:HD3	1:A:635:LEU:HB3	1.95	0.49
1:A:244:TRP:O	1:A:245:ALA:HB2	2.12	0.49
1:A:524:TYR:O	1:A:540:ILE:CD1	2.62	0.48
1:A:93:TYR:HB2	1:A:210:HIS:HB3	1.96	0.48
1:A:13:SER:HB2	1:A:15:PRO:HD2	1.96	0.48
1:A:198:LEU:HD23	1:A:203:GLY:O	2.14	0.48
1:A:87:GLY:O	1:A:88:SER:HB2	2.14	0.48
1:A:365:SER:HA	1:A:614:ARG:HH22	1.76	0.47
1:A:365:SER:HB2	1:A:368:ASP:HB2	1.96	0.47
1:A:391:ALA:HB2	1:A:604:ILE:HD13	1.95	0.47
1:A:532:VAL:HG21	1:A:561:LEU:HD21	1.96	0.47
1:A:529:ARG:HB2	1:A:557:TRP:CH2	2.49	0.47
1:A:192:SER:CB	1:A:296:LYS:HD2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:CG	1:A:292:ASP:N	2.78	0.47
1:A:460:ARG:O	1:A:465:VAL:HG23	2.15	0.47
1:A:605:ARG:NH1	1:A:647:VAL:O	2.48	0.47
1:A:415:TYR:OH	1:A:638:LYS:HE2	2.15	0.47
1:A:574:ARG:H	1:A:574:ARG:HD3	1.79	0.47
1:A:59:LEU:HD23	1:A:253:VAL:HG22	1.96	0.47
1:A:314:MET:HE1	1:A:683:LEU:HD21	1.96	0.47
1:A:361:TRP:O	1:A:364:VAL:HG12	2.15	0.47
1:A:492:SER:HB3	1:A:493:PRO:HD2	1.96	0.47
1:A:431:TYR:CE1	1:A:591:THR:HA	2.50	0.47
1:A:335:GLN:O	1:A:336:LEU:C	2.53	0.46
1:A:16:GLU:O	1:A:299:LEU:HD21	2.14	0.46
1:A:210:HIS:CD2	1:A:211:THR:HG22	2.50	0.46
1:A:376:GLU:HB2	1:A:379:ASP:OD2	2.16	0.46
1:A:520:LYS:HD3	1:A:529:ARG:NH1	2.31	0.46
1:A:509:PRO:O	1:A:510:PRO:O	2.34	0.46
1:A:47:LYS:HG2	1:A:72:TYR:CE1	2.51	0.46
1:A:432:PHE:N	1:A:432:PHE:CD1	2.83	0.46
1:A:49:ILE:CD1	1:A:57:ILE:HG22	2.46	0.46
1:A:461:THR:HG21	1:A:589:VAL:HG21	1.98	0.46
1:A:221:LYS:HE3	1:A:237:ASP:OD2	2.16	0.46
1:A:125:TRP:O	1:A:129:ILE:HG12	2.16	0.45
1:A:444:ASN:HD21	1:A:447:ASN:N	2.14	0.45
1:A:460:ARG:HB3	4:A:690:CO3:C	2.46	0.45
1:A:46:ILE:HG23	1:A:74:LEU:CD2	2.47	0.45
1:A:43:LEU:HG	1:A:47:LYS:HE3	1.97	0.45
1:A:92:TYR:O	1:A:246:ARG:HA	2.17	0.45
1:A:209:LYS:HZ3	1:A:301:LYS:NZ	2.09	0.45
1:A:290:LYS:O	1:A:291:LYS:CB	2.64	0.45
1:A:562:GLN:HE21	1:A:562:GLN:HB3	1.46	0.45
1:A:444:ASN:HD21	1:A:446:ASN:C	2.21	0.45
1:A:546:GLU:O	1:A:552:LYS:HD2	2.17	0.45
1:A:557:TRP:CD1	1:A:557:TRP:N	2.83	0.44
1:A:34:LEU:HG	1:A:35:THR:N	2.32	0.44
1:A:472:HIS:ND1	1:A:477:THR:O	2.50	0.44
1:A:24:ARG:HG3	1:A:34:LEU:O	2.18	0.44
1:A:84:HIS:HB2	1:A:88:SER:CA	2.44	0.44
1:A:334:ASP:OD2	1:A:335:GLN:N	2.51	0.44
1:A:129:ILE:O	1:A:133:LEU:HG	2.17	0.44
1:A:413:GLU:HG2	1:A:644:LEU:HD11	1.98	0.44
1:A:34:LEU:HD22	1:A:266:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:O	1:A:250:HIS:HB3	2.18	0.44
1:A:390:ASP:O	1:A:596:VAL:HG12	2.17	0.44
1:A:474:ARG:HB3	1:A:475:THR:H	1.68	0.44
1:A:267:LEU:O	1:A:271:GLN:HG3	2.18	0.44
1:A:12:ILE:O	1:A:13:SER:CB	2.64	0.44
1:A:42:TYR:CE2	1:A:63:GLN:HG2	2.52	0.44
1:A:240:LYS:HG3	5:A:702:HOH:O	2.19	0.43
1:A:578:VAL:HG12	1:A:578:VAL:O	2.18	0.43
1:A:6:VAL:HG23	1:A:6:VAL:O	2.19	0.43
1:A:443:VAL:HA	1:A:451:LYS:NZ	2.33	0.43
1:A:453:SER:O	1:A:487:GLY:CA	2.66	0.43
1:A:540:ILE:CG2	1:A:544:THR:HB	2.48	0.43
1:A:92:TYR:HE1	1:A:249:ALA:HA	1.84	0.43
1:A:93:TYR:O	1:A:209:LYS:HA	2.18	0.43
1:A:363:VAL:HG23	1:A:364:VAL:N	2.34	0.43
1:A:447:ASN:C	1:A:449:LYS:N	2.71	0.43
1:A:477:THR:CG2	1:A:478:CYS:N	2.80	0.43
1:A:509:PRO:O	1:A:509:PRO:HG2	2.19	0.43
1:A:18:LYS:HG2	1:A:22:ASN:HD21	1.84	0.43
1:A:46:ILE:HG23	1:A:74:LEU:HD21	2.00	0.43
1:A:49:ILE:HG13	1:A:54:ALA:HB3	2.01	0.43
1:A:553:ASN:ND2	1:A:555:ALA:N	2.66	0.43
1:A:59:LEU:CD2	1:A:253:VAL:HG22	2.48	0.43
1:A:89:THR:OG1	1:A:90:THR:N	2.50	0.43
1:A:444:ASN:ND2	1:A:444:ASN:C	2.71	0.43
1:A:8:ARG:HH22	1:A:52:ASN:C	2.23	0.42
1:A:14:SER:HB2	1:A:15:PRO:HD3	2.01	0.42
1:A:17:GLU:O	1:A:17:GLU:OE2	2.37	0.42
1:A:184:ARG:HG3	1:A:184:ARG:NH1	2.34	0.42
1:A:437:ALA:O	1:A:566:PHE:HA	2.19	0.42
1:A:291:LYS:CG	1:A:292:ASP:H	2.31	0.42
1:A:417:ASP:C	1:A:419:SER:H	2.23	0.42
1:A:37:VAL:O	1:A:37:VAL:HG12	2.20	0.42
1:A:72:TYR:HB3	1:A:74:LEU:CD2	2.49	0.42
1:A:153:ALA:HB2	1:A:167:GLU:HG2	1.97	0.42
1:A:16:GLU:CD	1:A:299:LEU:H	2.22	0.42
1:A:168:GLN:CD	1:A:168:GLN:H	2.21	0.42
1:A:216:ASN:O	1:A:290:LYS:HG3	2.20	0.42
1:A:355:LYS:HG3	1:A:359:ASP:OD1	2.20	0.42
1:A:586:LEU:O	1:A:587:ALA:HB2	2.20	0.42
1:A:92:TYR:CE1	1:A:249:ALA:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:THR:OG1	1:A:233:ARG:NH1	2.50	0.42
1:A:127:ILE:N	1:A:128:PRO:CD	2.83	0.42
1:A:524:TYR:CD1	1:A:541:GLN:HB2	2.55	0.42
1:A:640:LEU:HB2	5:A:698:HOH:O	2.18	0.42
1:A:259:LYS:O	1:A:261:GLU:N	2.53	0.42
1:A:458:VAL:CG2	1:A:492:SER:OG	2.62	0.42
1:A:564:ASP:C	1:A:566:PHE:H	2.22	0.42
1:A:412:ALA:HB3	1:A:645:PHE:CZ	2.55	0.42
1:A:455:HIS:CD2	1:A:489:ALA:HB2	2.55	0.42
1:A:32:ILE:HD12	1:A:32:ILE:N	2.18	0.42
1:A:65:PHE:CD1	1:A:65:PHE:C	2.93	0.42
1:A:510:PRO:O	1:A:511:GLU:CB	2.67	0.42
1:A:17:GLU:OE2	1:A:17:GLU:CA	2.68	0.41
1:A:524:TYR:HA	1:A:540:ILE:HD11	2.01	0.41
1:A:413:GLU:CA	1:A:644:LEU:HD12	2.47	0.41
1:A:59:LEU:N	1:A:59:LEU:HD22	2.35	0.41
1:A:339:SER:O	1:A:340:PRO:C	2.58	0.41
1:A:24:ARG:NH1	1:A:24:ARG:CG	2.79	0.41
1:A:430:SER:HB2	1:A:589:VAL:O	2.20	0.41
1:A:215:GLU:O	1:A:296:LYS:NZ	2.49	0.41
1:A:77:ILE:H	1:A:77:ILE:HG12	1.62	0.41
1:A:410:VAL:CG2	1:A:605:ARG:NH2	2.83	0.41
1:A:444:ASN:ND2	1:A:447:ASN:CB	2.80	0.41
1:A:11:THR:HG22	1:A:299:LEU:HD11	2.02	0.41
1:A:125:TRP:O	1:A:128:PRO:HD2	2.21	0.41
1:A:309:ARG:HG3	1:A:310:VAL:N	2.35	0.41
1:A:318:LEU:HD13	1:A:386:LYS:CE	2.46	0.41
1:A:464:TRP:O	1:A:467:PRO:HD2	2.21	0.41
1:A:464:TRP:CE2	1:A:468:MET:HG3	2.55	0.41
1:A:521:TYR:CD1	1:A:530:CYS:HB2	2.55	0.41
1:A:532:VAL:HG22	1:A:566:PHE:CZ	2.52	0.41
1:A:195:PHE:CD2	1:A:216:ASN:HB3	2.56	0.41
1:A:417:ASP:C	1:A:419:SER:N	2.74	0.41
1:A:305:ILE:O	1:A:306:MET:HG2	2.21	0.40
1:A:493:PRO:HB2	1:A:496:SER:CB	2.50	0.40
1:A:679:MET:SD	1:A:679:MET:C	3.00	0.40
1:A:21:ASN:O	1:A:22:ASN:C	2.57	0.40
1:A:435:ALA:CB	1:A:569:LEU:HB2	2.48	0.40
1:A:75:LYS:HA	1:A:76:PRO:HD3	1.93	0.40
1:A:82:TYR:CE2	1:A:249:ALA:CB	3.04	0.40
1:A:209:LYS:HE2	1:A:211:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:O	1:A:265:SER:HB2	2.20	0.40
1:A:448:LEU:HB3	1:A:484:PHE:HE1	1.86	0.40
1:A:486:GLU:HB3	1:A:500:GLN:NE2	2.37	0.40
1:A:493:PRO:HA	1:A:494:PRO:HD2	1.87	0.40
1:A:540:ILE:HG12	1:A:544:THR:HG21	2.03	0.40
1:A:291:LYS:HE2	1:A:291:LYS:HB3	1.83	0.40
1:A:432:PHE:HD2	1:A:585:ASN:ND2	2.19	0.40
1:A:317:GLN:HA	1:A:325:TYR:CD2	2.55	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	681/686 (99%)	562 (82%)	85 (12%)	34 (5%)	2 6

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	260	VAL
1	A	336	LEU
1	A	338	PRO
1	A	339	SER
1	A	341	ARG
1	A	343	ASN
1	A	508	ILE
1	A	510	PRO
1	A	571	THR
1	A	57	ILE
1	A	210	HIS
1	A	448	LEU

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Mol	Chain	Res	Type
1	A	511	GLU
1	A	534	LYS
1	A	540	ILE
1	A	620	SER
1	A	242	CYS
1	A	291	LYS
1	A	337	THR
1	A	490	PRO
1	A	558	ALA
1	A	684	GLU
1	A	87	GLY
1	A	461	THR
1	A	465	VAL
1	A	88	SER
1	A	162	PRO
1	A	288	PRO
1	A	493	PRO
1	A	666	SER
1	A	236	VAL
1	A	467	PRO
1	A	450	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	561/580 (97%)	505 (90%)	56 (10%)	7 22

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	32	ILE
1	A	35	THR
1	A	69	LEU
1	A	74	LEU

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Mol	Chain	Res	Type
1	A	77	ILE
1	A	89	THR
1	A	132	LEU
1	A	141	GLU
1	A	154	LYS
1	A	168	GLN
1	A	172	ARG
1	A	182	CYS
1	A	184	ARG
1	A	185	ASN
1	A	198	LEU
1	A	205	VAL
1	A	211	THR
1	A	215	GLU
1	A	258	ASN
1	A	309	ARG
1	A	318	LEU
1	A	323	GLU
1	A	333	LYS
1	A	338	PRO
1	A	340	PRO
1	A	343	ASN
1	A	344	ARG
1	A	410	VAL
1	A	438	ARG
1	A	444	ASN
1	A	447	ASN
1	A	510	PRO
1	A	512	LYS
1	A	513	CYS
1	A	528	LEU
1	A	534	LYS
1	A	540	ILE
1	A	553	ASN
1	A	557	TRP
1	A	560	ASN
1	A	562	GLN
1	A	574	ARG
1	A	577	ASN
1	A	597	ARG
1	A	603	LYS
1	A	604	ILE

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Mol	Chain	Res	Type
1	A	635	LEU
1	A	636	LEU
1	A	640	LEU
1	A	644	LEU
1	A	660	LYS
1	A	663	THR
1	A	665	ILE
1	A	668	LEU
1	A	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	22	ASN
1	A	28	GLN
1	A	52	ASN
1	A	63	GLN
1	A	84	HIS
1	A	185	ASN
1	A	220	GLN
1	A	258	ASN
1	A	283	HIS
1	A	444	ASN
1	A	479	ASN
1	A	500	GLN
1	A	542	HIS
1	A	548	ASN
1	A	553	ASN
1	A	562	GLN
1	A	577	ASN
1	A	672	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FUL	A	691	-	11,11,11	0.69	0	15,16,16	1.79	2 (13%)
4	CO3	A	689	3	2,3,3	0.35	0	2,3,3	0.02	0
4	CO3	A	690	3	2,3,3	0.25	0	2,3,3	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUL	A	691	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	691	FUL	C3-C4-C5	5.39	118.16	109.77
2	A	691	FUL	C4-C3-C2	3.22	116.44	110.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	691	FUL	4	0
4	A	690	CO3	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	683/686 (99%)	-0.44	11 (1%)	72	66	11, 37, 69, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.9
1	A	335	GLN	3.6
1	A	508	ILE	3.2
1	A	422	SER	3.1
1	A	336	LEU	2.6
1	A	425	ASP	2.5
1	A	289	GLY	2.4
1	A	339	SER	2.2
1	A	572	ASP	2.2
1	A	87	GLY	2.1
1	A	424	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUL	A	691	11/11	0.83	0.45	20,20,20,20	11
4	CO3	A	690	4/4	0.97	0.15	38,38,38,38	0
3	FE	A	688	1/1	0.99	0.09	35,35,35,35	0
4	CO3	A	689	4/4	0.99	0.12	29,29,29,29	0
3	FE	A	687	1/1	0.99	0.06	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.