Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:09 PM GMT

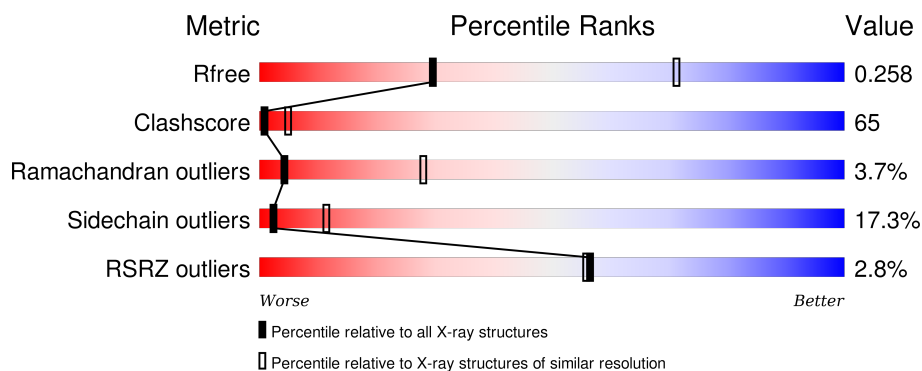|		
PDB ID	:	1NQG
Title	:	OUTER MEMBRANE COBALAMIN TRANSPORTER (BTUB) FROM E. COLI, WITH BOUND CALCIUM
Authors	:	Chimento, D.P.; Mohanty, A.K.; Kadner, R.J.; Wiener, M.C.
Deposited on	:	2003-01-21
Resolution	:	3.31 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		65
Ramachandran outliers		3.7%
Sidechain outliers		17.3%
RSRZ outliers		2.8%

Worse *Better*

▮ Percentile relative to all X-ray structures
◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	594	3% ▮ 40% 39% 16% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	800	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	C8E	A	801	-	-	-	X
3	C8E	A	803	-	-	-	X
3	C8E	A	804	-	-	-	X
3	C8E	A	805	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4685 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 vitamin b12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total 4555	C 2863	N 781	O 909	S 2	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Ca 4	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0

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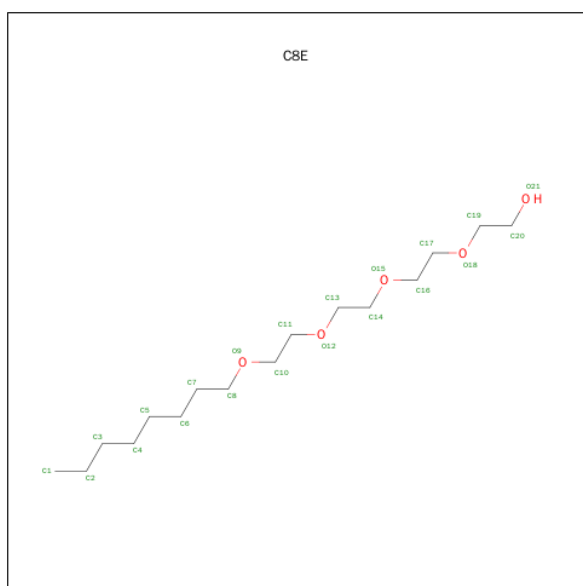
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: vitamin b12 receptor
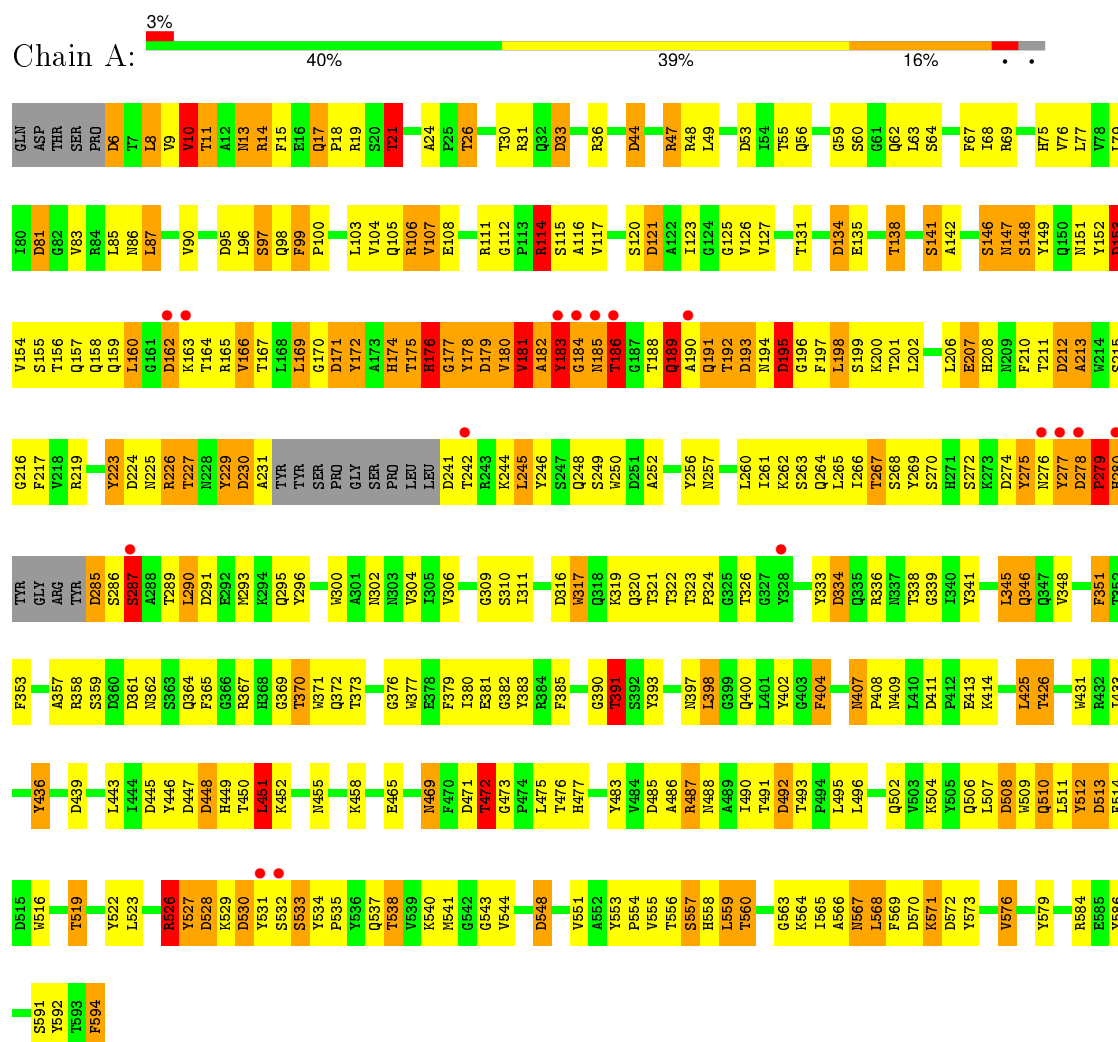
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.63Å 81.63Å 225.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.31 30.27 – 3.31	Depositor EDS
% Data completeness (in resolution range)	95.1 (20.00-3.31) 95.0 (30.27-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	8.68 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.234 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	642 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.8	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 13009 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, C8E

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	1.37	16/4666 (0.3%)	1.42	44/6352 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	TRP	CB-CG	-7.77	1.36	1.50
1	A	317	TRP	CB-CG	-7.18	1.37	1.50
1	A	306	VAL	CA-CB	-6.12	1.42	1.54
1	A	436	TYR	CB-CG	-5.96	1.42	1.51
1	A	311	ILE	CA-CB	-5.62	1.42	1.54
1	A	576	VAL	CB-CG1	-5.61	1.41	1.52
1	A	10	VAL	CA-CB	-5.43	1.43	1.54
1	A	310	SER	CB-OG	-5.29	1.35	1.42
1	A	17	GLN	CB-CG	-5.21	1.38	1.52
1	A	351	PHE	CB-CG	-5.11	1.42	1.51
1	A	83	VAL	CA-CB	-5.09	1.44	1.54
1	A	483	TYR	CD2-CE2	-5.09	1.31	1.39
1	A	573	TYR	CD1-CE1	-5.08	1.31	1.39
1	A	99	PHE	CE1-CZ	-5.08	1.27	1.37
1	A	377	TRP	CG-CD1	-5.05	1.29	1.36
1	A	117	VAL	CA-CB	-5.04	1.44	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	LEU	CB-CG-CD1	-9.57	94.72	111.00
1	A	487	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	A	106	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	81	ASP	CB-CG-OD2	8.81	126.23	118.30
1	A	492	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	570	ASP	CB-CG-OD2	7.96	125.46	118.30
1	A	230	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	193	ASP	CB-CG-OD2	7.63	125.17	118.30
1	A	195	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	134	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	274	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	361	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	114	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	528	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	530	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	526	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	485	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	548	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	306	VAL	CB-CA-C	-6.26	99.51	111.40
1	A	508	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	171	ASP	CB-CG-OD2	6.01	123.70	118.30
1	A	512	TYR	CB-CA-C	5.97	122.34	110.40
1	A	85	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	A	563	GLY	N-CA-C	-5.82	98.54	113.10
1	A	134	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	A	21	THR	OG1-CB-CG2	-5.71	96.86	110.00
1	A	44	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	513	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	472	THR	CB-CA-C	-5.54	96.64	111.60
1	A	334	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	153	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	316	ASP	N-CA-CB	-5.40	100.88	110.60
1	A	391	THR	N-CA-CB	-5.34	100.15	110.30
1	A	177	GLY	N-CA-C	5.32	126.40	113.10
1	A	166	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	6	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	445	ASP	CB-CA-C	-5.20	100.00	110.40
1	A	212	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	439	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	53	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	33	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	76	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	107	VAL	CB-CA-C	-5.06	101.79	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	TYR	CB-CG-CD1	-5.04	117.97	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	TYR	Peptide
1	A	279	PRO	Peptide
1	A	472	THR	Mainchain

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	4555	0	4272	574	0
2	A	4	0	0	0	0
3	A	126	0	204	37	0
All	All	4685	0	4476	591	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 65.

All (591) 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:278:ASP:CG	1:A:279:PRO:HA	1.27	1.48
1:A:181:VAL:CG1	1:A:182:ALA:H	1.29	1.44
1:A:244:LYS:HE3	1:A:246:TYR:CZ	1.59	1.38
1:A:358:ARG:O	3:A:800:C8E:H72	1.33	1.29
1:A:510:GLN:N	1:A:510:GLN:HE21	1.36	1.23
1:A:190:ALA:O	1:A:191:GLN:HG2	1.37	1.22
1:A:142:ALA:HB1	1:A:151:ASN:O	1.36	1.22
1:A:527:TYR:CZ	1:A:540:LYS:HD2	1.74	1.21
1:A:510:GLN:N	1:A:510:GLN:NE2	1.89	1.21
1:A:555:VAL:HG12	1:A:556:THR:HG23	1.24	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:182:ALA:N	1.30	1.19
1:A:226:ARG:NH1	1:A:244:LYS:NZ	1.91	1.17
1:A:278:ASP:CG	1:A:279:PRO:CA	2.12	1.16
1:A:226:ARG:NH1	1:A:244:LYS:CE	2.08	1.16
1:A:398:LEU:H	1:A:398:LEU:CD2	1.59	1.16
1:A:226:ARG:NH1	1:A:244:LYS:HZ3	1.42	1.15
1:A:309:GLY:HA3	1:A:346:GLN:NE2	1.63	1.13
1:A:162:ASP:C	1:A:163:LYS:HG2	1.68	1.12
1:A:169:LEU:HD13	1:A:170:GLY:N	1.62	1.12
1:A:286:SER:O	1:A:287:SER:HB2	1.44	1.12
1:A:277:TYR:HB2	1:A:278:ASP:HB3	1.32	1.11
1:A:527:TYR:OH	1:A:540:LYS:HD2	1.50	1.11
1:A:278:ASP:HB2	1:A:279:PRO:C	1.71	1.10
1:A:181:VAL:CG1	1:A:182:ALA:N	1.94	1.10
1:A:278:ASP:OD1	1:A:279:PRO:HA	1.50	1.09
1:A:290:LEU:HD12	1:A:290:LEU:C	1.70	1.09
1:A:180:VAL:HG23	1:A:180:VAL:O	1.51	1.09
1:A:277:TYR:HB2	1:A:278:ASP:CB	1.82	1.09
1:A:278:ASP:CB	1:A:279:PRO:HA	1.83	1.08
1:A:509:TRP:C	1:A:510:GLN:HE21	1.56	1.08
1:A:491:THR:HG23	1:A:493:THR:HG23	1.09	1.07
1:A:277:TYR:HB2	1:A:278:ASP:CA	1.84	1.07
1:A:244:LYS:CE	1:A:246:TYR:CZ	2.37	1.07
1:A:77:LEU:HD21	1:A:79:LEU:HD21	1.31	1.07
1:A:398:LEU:H	1:A:398:LEU:HD23	1.09	1.06
1:A:451:LEU:N	1:A:451:LEU:HD22	1.63	1.06
1:A:190:ALA:O	1:A:191:GLN:CG	2.03	1.05
1:A:509:TRP:C	1:A:510:GLN:NE2	2.09	1.05
1:A:189:GLN:HA	1:A:189:GLN:OE1	1.57	1.05
1:A:506:GLN:NE2	1:A:519:THR:HB	1.72	1.04
1:A:226:ARG:HH12	1:A:244:LYS:HE2	1.18	1.04
1:A:278:ASP:CB	1:A:279:PRO:CA	2.35	1.03
1:A:226:ARG:HH11	1:A:244:LYS:NZ	1.50	1.02
1:A:446:TYR:OH	1:A:451:LEU:HD13	1.60	1.01
1:A:189:GLN:CA	1:A:189:GLN:OE1	2.09	1.00
1:A:555:VAL:HG12	1:A:556:THR:CG2	1.92	0.99
1:A:172:TYR:HD2	1:A:172:TYR:O	1.43	0.99
1:A:397:ASN:H	1:A:400:GLN:HE21	1.08	0.99
1:A:162:ASP:O	1:A:163:LYS:CG	2.10	0.99
1:A:527:TYR:CE1	1:A:540:LYS:HG3	1.97	0.98
1:A:169:LEU:CD1	1:A:169:LEU:C	2.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:CD2	1:A:172:TYR:O	2.17	0.98
1:A:160:LEU:HD22	1:A:166:VAL:HG21	1.42	0.98
1:A:397:ASN:H	1:A:400:GLN:NE2	1.62	0.97
1:A:244:LYS:HE3	1:A:246:TYR:CE1	1.99	0.97
1:A:278:ASP:HB2	1:A:279:PRO:O	1.62	0.97
1:A:527:TYR:OH	1:A:540:LYS:HE3	1.63	0.97
1:A:165:ARG:HG3	1:A:207:GLU:OE1	1.63	0.97
1:A:186:THR:HA	1:A:231:ALA:HB2	1.47	0.97
1:A:527:TYR:OH	1:A:540:LYS:CD	2.13	0.95
1:A:226:ARG:NH1	1:A:244:LYS:HE2	1.76	0.95
1:A:534:TYR:CG	1:A:535:PRO:HA	2.00	0.95
1:A:142:ALA:HB2	1:A:152:TYR:HA	1.47	0.94
1:A:527:TYR:OH	1:A:540:LYS:CE	2.16	0.94
1:A:379:PHE:O	1:A:380:ILE:HG13	1.67	0.94
1:A:160:LEU:HD22	1:A:166:VAL:CG2	1.96	0.94
1:A:77:LEU:CD2	1:A:79:LEU:HD21	1.98	0.93
1:A:290:LEU:HD12	1:A:291:ASP:N	1.83	0.93
1:A:526:ARG:HD3	1:A:541:MET:HE1	1.50	0.93
1:A:398:LEU:N	1:A:398:LEU:CD2	2.27	0.93
1:A:120:SER:HB2	1:A:393:TYR:CE1	2.03	0.93
1:A:169:LEU:C	1:A:169:LEU:HD13	1.87	0.92
1:A:184:GLY:H	1:A:532:SER:CB	1.75	0.92
1:A:323:THR:HG22	1:A:324:PRO:O	1.68	0.92
1:A:451:LEU:H	1:A:451:LEU:HD22	1.30	0.92
1:A:446:TYR:OH	1:A:451:LEU:CD1	2.16	0.91
1:A:451:LEU:N	1:A:451:LEU:CD2	2.32	0.91
1:A:491:THR:CG2	1:A:493:THR:HG23	2.00	0.91
1:A:114:ARG:HA	1:A:372:GLN:HE22	1.33	0.91
1:A:10:VAL:HG12	1:A:11:THR:N	1.82	0.91
1:A:510:GLN:CA	1:A:510:GLN:HE21	1.83	0.90
1:A:190:ALA:O	1:A:191:GLN:NE2	2.04	0.89
1:A:197:PHE:CD2	1:A:227:THR:CG2	2.56	0.89
1:A:184:GLY:H	1:A:532:SER:HB3	1.37	0.89
1:A:358:ARG:O	3:A:800:C8E:C7	2.20	0.88
1:A:404:PHE:O	1:A:404:PHE:HD2	1.56	0.88
1:A:142:ALA:CB	1:A:151:ASN:O	2.19	0.88
1:A:411:ASP:H	1:A:455:ASN:HD21	1.17	0.88
1:A:226:ARG:HH11	1:A:244:LYS:HZ3	0.91	0.87
1:A:244:LYS:CE	1:A:246:TYR:OH	2.22	0.87
1:A:165:ARG:O	1:A:207:GLU:OE1	1.93	0.87
1:A:174:HIS:CD2	1:A:174:HIS:C	2.48	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:HB2	1:A:279:PRO:CA	2.00	0.86
1:A:278:ASP:O	1:A:280:HIS:CD2	2.28	0.86
1:A:472:THR:OG1	1:A:472:THR:O	1.88	0.86
1:A:197:PHE:HD2	1:A:227:THR:CG2	1.89	0.85
1:A:275:TYR:CE2	1:A:290:LEU:HD22	2.10	0.85
1:A:244:LYS:HE3	1:A:246:TYR:OH	1.76	0.85
1:A:162:ASP:C	1:A:163:LYS:CG	2.43	0.84
1:A:319:LYS:HE3	1:A:336:ARG:NH2	1.92	0.84
1:A:426:THR:CG2	1:A:431:TRP:HE1	1.90	0.84
1:A:8:LEU:O	1:A:8:LEU:CD1	2.26	0.83
1:A:263:SER:OG	1:A:302:ASN:ND2	2.11	0.83
1:A:162:ASP:O	1:A:163:LYS:HG2	1.70	0.83
1:A:286:SER:O	1:A:287:SER:CB	2.27	0.82
1:A:425:LEU:CD2	1:A:425:LEU:C	2.47	0.82
1:A:189:GLN:N	1:A:189:GLN:OE1	2.13	0.82
1:A:488:ASN:N	1:A:495:LEU:HD21	1.94	0.82
1:A:290:LEU:CD1	1:A:290:LEU:C	2.47	0.82
1:A:362:ASN:ND2	1:A:364:GLN:H	1.75	0.81
1:A:556:THR:OG1	1:A:557:SER:N	2.13	0.81
1:A:317:TRP:HD1	1:A:338:THR:OG1	1.62	0.81
1:A:425:LEU:HD23	1:A:425:LEU:C	2.01	0.81
1:A:277:TYR:CB	1:A:278:ASP:HB3	2.09	0.81
1:A:192:THR:O	1:A:192:THR:HG22	1.80	0.80
1:A:277:TYR:HB2	1:A:278:ASP:HA	1.63	0.80
1:A:279:PRO:O	1:A:280:HIS:O	1.99	0.80
1:A:280:HIS:CE1	1:A:285:ASP:OD2	2.34	0.80
1:A:81:ASP:OD2	1:A:131:THR:OG1	1.99	0.80
1:A:527:TYR:CZ	1:A:540:LYS:CD	2.61	0.80
1:A:24:ALA:O	1:A:26:THR:HG22	1.81	0.80
1:A:506:GLN:HE22	1:A:519:THR:HB	1.40	0.80
1:A:172:TYR:C	1:A:172:TYR:CD2	2.54	0.80
1:A:180:VAL:CG2	1:A:180:VAL:O	2.25	0.80
1:A:226:ARG:HD2	1:A:244:LYS:HG3	1.62	0.80
1:A:13:ASN:O	1:A:14:ARG:HB2	1.81	0.79
1:A:279:PRO:C	1:A:280:HIS:O	2.20	0.79
1:A:369:GLY:HA3	3:A:800:C8E:H82	1.64	0.78
1:A:56:GLN:HG3	1:A:64:SER:HB3	1.66	0.78
1:A:197:PHE:CD2	1:A:227:THR:HG22	2.18	0.78
1:A:197:PHE:HD2	1:A:227:THR:CB	1.95	0.78
1:A:280:HIS:HE1	1:A:285:ASP:OD2	1.65	0.78
1:A:226:ARG:HH11	1:A:244:LYS:CE	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:N	1:A:398:LEU:HD22	1.98	0.77
1:A:516:TRP:CE3	1:A:551:VAL:CG1	2.66	0.77
1:A:527:TYR:CE1	1:A:540:LYS:CG	2.67	0.77
1:A:81:ASP:OD2	1:A:219:ARG:NH1	2.18	0.77
1:A:191:GLN:HB3	1:A:230:ASP:OD2	1.84	0.77
1:A:278:ASP:C	1:A:280:HIS:HD2	1.87	0.76
1:A:527:TYR:HE1	1:A:540:LYS:HG3	1.46	0.76
1:A:162:ASP:O	1:A:163:LYS:HG3	1.85	0.76
1:A:190:ALA:C	1:A:191:GLN:HG2	2.05	0.76
1:A:186:THR:CA	1:A:231:ALA:HB2	2.16	0.76
1:A:95:ASP:OD1	1:A:97:SER:HB3	1.86	0.76
1:A:446:TYR:CZ	1:A:451:LEU:HA	2.21	0.75
1:A:148:SER:O	1:A:148:SER:OG	2.05	0.75
1:A:245:LEU:CD2	1:A:246:TYR:N	2.49	0.75
1:A:169:LEU:C	1:A:169:LEU:HD12	2.05	0.75
1:A:179:ASP:HA	1:A:195:ASP:OD2	1.87	0.75
1:A:358:ARG:C	3:A:800:C8E:H72	2.05	0.75
1:A:160:LEU:CD2	1:A:166:VAL:HG21	2.17	0.75
1:A:186:THR:N	1:A:231:ALA:HB1	2.03	0.74
1:A:534:TYR:CD1	1:A:535:PRO:CA	2.70	0.74
1:A:309:GLY:CA	1:A:346:GLN:NE2	2.45	0.74
1:A:506:GLN:HE22	1:A:519:THR:CB	1.99	0.74
1:A:186:THR:H	1:A:231:ALA:HB1	1.51	0.74
1:A:527:TYR:CD1	1:A:527:TYR:N	2.54	0.74
1:A:142:ALA:CB	1:A:152:TYR:HA	2.17	0.73
1:A:174:HIS:CD2	1:A:174:HIS:O	2.41	0.73
1:A:407:ASN:C	1:A:407:ASN:HD22	1.89	0.73
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.52	0.73
1:A:13:ASN:C	1:A:13:ASN:HD22	1.92	0.73
1:A:186:THR:N	1:A:231:ALA:CB	2.52	0.72
1:A:277:TYR:N	1:A:277:TYR:CD2	2.55	0.72
1:A:527:TYR:CE1	1:A:540:LYS:HD2	2.21	0.72
1:A:8:LEU:HD12	1:A:8:LEU:O	1.90	0.72
1:A:186:THR:HA	1:A:231:ALA:CB	2.18	0.71
1:A:8:LEU:HD13	1:A:8:LEU:O	1.90	0.71
1:A:13:ASN:ND2	1:A:15:PHE:H	1.87	0.71
1:A:245:LEU:HD23	1:A:246:TYR:N	2.06	0.71
1:A:526:ARG:HD3	1:A:541:MET:CE	2.19	0.71
1:A:487:ARG:NH1	1:A:492:ASP:O	2.23	0.71
1:A:153:ASP:HB2	1:A:171:ASP:OD1	1.89	0.71
1:A:371:TRP:CE2	3:A:805:C8E:H62	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLU:HG3	1:A:382:GLY:N	2.06	0.70
1:A:126:VAL:CG1	1:A:127:VAL:N	2.53	0.70
1:A:277:TYR:H	1:A:277:TYR:HD2	1.33	0.70
1:A:357:ALA:HB1	3:A:800:C8E:H52	1.73	0.70
1:A:175:THR:O	1:A:176:HIS:C	2.27	0.70
1:A:244:LYS:HE2	1:A:246:TYR:OH	1.90	0.70
1:A:135:GLU:H	1:A:157:GLN:HE22	1.39	0.70
1:A:114:ARG:HA	1:A:372:GLN:NE2	2.06	0.70
1:A:373:THR:HG21	3:A:803:C8E:H131	1.74	0.70
1:A:357:ALA:HB2	3:A:805:C8E:H13	1.74	0.70
1:A:526:ARG:CD	1:A:541:MET:CE	2.69	0.70
1:A:278:ASP:HB2	1:A:280:HIS:O	1.92	0.69
1:A:526:ARG:CD	1:A:541:MET:HE1	2.22	0.69
1:A:149:TYR:HA	1:A:175:THR:HB	1.74	0.69
3:A:802:C8E:H52	3:A:802:C8E:H13	1.72	0.69
1:A:201:THR:HG22	1:A:202:LEU:N	2.06	0.69
1:A:277:TYR:CB	1:A:278:ASP:CA	2.69	0.69
1:A:527:TYR:CE1	1:A:540:LYS:CD	2.76	0.69
1:A:511:LEU:HD21	1:A:512:TYR:CE2	2.27	0.69
1:A:185:ASN:O	1:A:186:THR:HB	1.93	0.69
1:A:197:PHE:CD2	1:A:227:THR:HB	2.27	0.69
1:A:190:ALA:O	1:A:191:GLN:CD	2.31	0.69
1:A:197:PHE:HD2	1:A:227:THR:HB	1.58	0.69
1:A:277:TYR:N	1:A:277:TYR:HD2	1.91	0.69
1:A:534:TYR:CD1	1:A:535:PRO:HA	2.28	0.69
3:A:802:C8E:H11	3:A:802:C8E:H171	1.75	0.69
1:A:511:LEU:HG	1:A:512:TYR:N	2.06	0.68
1:A:450:THR:O	1:A:451:LEU:C	2.32	0.68
1:A:527:TYR:HD1	1:A:527:TYR:N	1.90	0.67
1:A:491:THR:HG23	1:A:493:THR:CG2	2.05	0.67
1:A:407:ASN:ND2	1:A:409:ASN:H	1.91	0.67
1:A:77:LEU:CG	1:A:79:LEU:HD21	2.24	0.67
1:A:506:GLN:HE21	1:A:519:THR:HB	1.59	0.67
1:A:291:ASP:HA	1:A:326:THR:HG23	1.76	0.67
1:A:534:TYR:CG	1:A:535:PRO:CA	2.75	0.67
1:A:370:THR:N	3:A:800:C8E:H81	2.10	0.67
1:A:47:ARG:NH2	1:A:548:ASP:OD2	2.27	0.67
1:A:516:TRP:CE3	1:A:551:VAL:HG13	2.29	0.67
1:A:275:TYR:CE2	1:A:290:LEU:CD2	2.77	0.67
1:A:185:ASN:O	1:A:186:THR:CB	2.43	0.66
1:A:197:PHE:CD2	1:A:227:THR:CB	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASP:OD2	1:A:47:ARG:NH1	2.28	0.66
1:A:165:ARG:HG3	1:A:207:GLU:CD	2.15	0.66
1:A:183:TYR:O	1:A:185:ASN:OD1	2.12	0.66
1:A:90:VAL:HG22	1:A:293:MET:HE3	1.76	0.66
1:A:371:TRP:CD2	3:A:805:C8E:H51	2.31	0.66
1:A:446:TYR:OH	1:A:451:LEU:HA	1.94	0.66
1:A:184:GLY:N	1:A:532:SER:CB	2.51	0.66
1:A:229:TYR:CZ	1:A:241:ASP:HB3	2.31	0.66
1:A:290:LEU:CD1	1:A:291:ASP:N	2.59	0.65
1:A:506:GLN:HE22	1:A:519:THR:CG2	2.10	0.65
1:A:229:TYR:O	1:A:230:ASP:OD1	2.14	0.65
1:A:181:VAL:HG13	1:A:182:ALA:N	2.09	0.65
1:A:291:ASP:CA	1:A:326:THR:HG23	2.27	0.65
1:A:191:GLN:O	1:A:193:ASP:N	2.28	0.65
1:A:529:LYS:NZ	1:A:538:THR:HG23	2.11	0.65
1:A:404:PHE:C	1:A:404:PHE:HD2	2.00	0.65
1:A:112:GLY:O	1:A:125:GLY:HA2	1.97	0.65
1:A:8:LEU:HD12	1:A:8:LEU:H	1.62	0.64
1:A:90:VAL:CG2	1:A:293:MET:HE3	2.27	0.64
1:A:104:VAL:C	1:A:105:GLN:HE21	2.01	0.64
1:A:397:ASN:OD1	1:A:400:GLN:HG3	1.97	0.64
1:A:291:ASP:CB	1:A:326:THR:HG23	2.27	0.64
1:A:176:HIS:HA	1:A:196:GLY:CA	2.28	0.64
1:A:397:ASN:N	1:A:400:GLN:HE21	1.90	0.64
1:A:165:ARG:C	1:A:207:GLU:OE1	2.35	0.64
1:A:186:THR:CA	1:A:231:ALA:CB	2.75	0.64
1:A:370:THR:OG1	1:A:391:THR:HG22	1.97	0.64
1:A:506:GLN:NE2	1:A:519:THR:CB	2.53	0.64
1:A:317:TRP:CD1	1:A:338:THR:OG1	2.49	0.64
1:A:245:LEU:HD22	1:A:246:TYR:N	2.12	0.64
1:A:309:GLY:HA3	1:A:346:GLN:HE22	1.62	0.64
1:A:153:ASP:OD1	1:A:153:ASP:C	2.36	0.64
1:A:55:THR:HB	1:A:576:VAL:CG2	2.27	0.64
1:A:458:LYS:HD2	1:A:490:ILE:HD11	1.78	0.64
1:A:227:THR:O	1:A:227:THR:OG1	2.16	0.63
1:A:516:TRP:CZ3	1:A:551:VAL:CG1	2.82	0.63
1:A:146:SER:OG	1:A:586:TYR:HB2	1.98	0.63
1:A:169:LEU:HD12	1:A:169:LEU:O	1.96	0.63
1:A:250:TRP:N	1:A:269:TYR:O	2.31	0.63
1:A:245:LEU:HD23	1:A:246:TYR:H	1.63	0.63
1:A:398:LEU:N	1:A:398:LEU:HD23	1.94	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:TYR:CD1	1:A:535:PRO:HG3	2.34	0.62
1:A:197:PHE:CE2	1:A:227:THR:CG2	2.82	0.62
1:A:226:ARG:CD	1:A:244:LYS:HZ3	2.12	0.62
1:A:526:ARG:C	1:A:527:TYR:HD1	2.03	0.62
1:A:162:ASP:HB2	1:A:163:LYS:HZ3	1.65	0.62
1:A:169:LEU:HD13	1:A:170:GLY:CA	2.28	0.62
1:A:425:LEU:HD23	1:A:426:THR:N	2.14	0.62
1:A:226:ARG:CZ	1:A:244:LYS:HZ3	2.10	0.62
1:A:404:PHE:C	1:A:404:PHE:CD2	2.72	0.62
1:A:323:THR:HG23	1:A:324:PRO:HD2	1.82	0.62
1:A:188:THR:C	1:A:189:GLN:OE1	2.38	0.62
1:A:278:ASP:C	1:A:280:HIS:CD2	2.72	0.62
1:A:36:ARG:NH1	1:A:508:ASP:OD1	2.33	0.61
1:A:224:ASP:C	1:A:224:ASP:OD1	2.37	0.61
1:A:309:GLY:HA3	1:A:346:GLN:HE21	1.59	0.61
1:A:13:ASN:C	1:A:13:ASN:ND2	2.52	0.61
1:A:592:TYR:HE1	1:A:594:PHE:CG	2.18	0.61
1:A:362:ASN:CB	1:A:365:PHE:CE2	2.83	0.61
1:A:477:HIS:CE1	1:A:507:LEU:HD11	2.36	0.61
1:A:555:VAL:CG1	1:A:556:THR:CG2	2.74	0.61
1:A:31:ARG:O	1:A:31:ARG:HD3	2.01	0.61
1:A:567:ASN:O	1:A:584:ARG:HB2	2.01	0.61
1:A:278:ASP:O	1:A:280:HIS:HD2	1.75	0.60
1:A:224:ASP:OD1	1:A:226:ARG:HD3	2.01	0.60
1:A:533:SER:O	1:A:535:PRO:O	2.20	0.60
1:A:115:SER:O	1:A:358:ARG:HD3	2.02	0.60
1:A:534:TYR:CE1	1:A:535:PRO:HG3	2.37	0.60
1:A:212:ASP:O	1:A:213:ALA:HB2	2.02	0.60
1:A:90:VAL:HA	1:A:293:MET:HE3	1.84	0.60
1:A:126:VAL:HG12	1:A:127:VAL:N	2.14	0.59
1:A:177:GLY:C	1:A:194:ASN:HB3	2.23	0.59
3:A:802:C8E:H161	3:A:802:C8E:H12	1.85	0.59
1:A:179:ASP:OD1	1:A:192:THR:HA	2.03	0.59
1:A:245:LEU:C	1:A:245:LEU:CD2	2.70	0.59
3:A:802:C8E:C17	3:A:802:C8E:H11	2.32	0.59
1:A:241:ASP:OD1	1:A:277:TYR:O	2.21	0.58
1:A:407:ASN:HD22	1:A:408:PRO:N	2.00	0.58
1:A:534:TYR:HA	1:A:535:PRO:C	2.24	0.58
1:A:534:TYR:CD2	1:A:535:PRO:HA	2.37	0.58
1:A:488:ASN:HB3	1:A:491:THR:HG22	1.85	0.58
1:A:181:VAL:HG12	1:A:182:ALA:H	0.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:O	1:A:212:ASP:OD2	2.22	0.58
1:A:30:THR:O	1:A:33:ASP:HB2	2.04	0.58
1:A:77:LEU:HD11	1:A:79:LEU:CD2	2.34	0.58
1:A:472:THR:O	1:A:475:LEU:HB2	2.04	0.58
1:A:362:ASN:CG	1:A:365:PHE:CE2	2.77	0.58
1:A:201:THR:CG2	1:A:202:LEU:N	2.66	0.57
1:A:446:TYR:OH	1:A:451:LEU:HD12	2.00	0.57
1:A:371:TRP:CZ2	3:A:805:C8E:H62	2.39	0.57
1:A:526:ARG:HG2	1:A:541:MET:HE2	1.86	0.57
1:A:407:ASN:ND2	1:A:407:ASN:C	2.53	0.57
1:A:277:TYR:CB	1:A:278:ASP:HA	2.32	0.57
1:A:197:PHE:HD2	1:A:227:THR:HG22	1.56	0.57
1:A:19:ARG:NH2	1:A:26:THR:O	2.37	0.57
1:A:77:LEU:CG	1:A:79:LEU:CD2	2.82	0.57
1:A:160:LEU:CD2	1:A:166:VAL:CG2	2.79	0.57
1:A:296:TYR:HB2	1:A:319:LYS:HB3	1.87	0.57
1:A:226:ARG:HH11	1:A:244:LYS:CD	2.18	0.57
1:A:176:HIS:HA	1:A:196:GLY:HA2	1.86	0.57
3:A:803:C8E:H172	3:A:803:C8E:C10	2.34	0.57
1:A:116:ALA:HB2	1:A:370:THR:HG23	1.86	0.57
1:A:362:ASN:HD22	1:A:364:GLN:H	1.50	0.57
1:A:175:THR:O	1:A:176:HIS:O	2.23	0.57
1:A:197:PHE:CE2	1:A:227:THR:HG22	2.39	0.56
1:A:357:ALA:CB	3:A:800:C8E:H52	2.34	0.56
1:A:526:ARG:CG	1:A:541:MET:HE2	2.34	0.56
1:A:516:TRP:CZ3	1:A:551:VAL:HG11	2.40	0.56
1:A:502:GLN:HG2	1:A:523:LEU:HD23	1.86	0.56
1:A:341:TYR:C	1:A:341:TYR:CD1	2.79	0.56
1:A:556:THR:HG1	1:A:558:HIS:H	1.51	0.56
1:A:534:TYR:CE1	1:A:535:PRO:HB3	2.40	0.56
1:A:594:PHE:N	1:A:594:PHE:CD1	2.73	0.56
1:A:166:VAL:HG12	1:A:167:THR:N	2.21	0.56
1:A:323:THR:HG22	1:A:324:PRO:N	2.22	0.55
1:A:135:GLU:H	1:A:157:GLN:NE2	2.04	0.55
1:A:162:ASP:HB2	1:A:163:LYS:NZ	2.20	0.55
1:A:142:ALA:HB2	1:A:152:TYR:CA	2.30	0.55
1:A:185:ASN:O	1:A:186:THR:HG22	2.07	0.55
1:A:383:TYR:OH	1:A:426:THR:HB	2.06	0.55
1:A:249:SER:HA	1:A:270:SER:HA	1.87	0.55
1:A:371:TRP:CG	3:A:805:C8E:H51	2.42	0.55
1:A:425:LEU:HD22	1:A:425:LEU:C	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLY:N	1:A:532:SER:HB3	2.13	0.55
1:A:369:GLY:CA	3:A:800:C8E:H82	2.35	0.55
1:A:69:ARG:HD3	1:A:436:TYR:CE1	2.42	0.55
1:A:357:ALA:CB	3:A:805:C8E:H13	2.37	0.55
1:A:379:PHE:C	1:A:380:ILE:HG13	2.25	0.55
1:A:309:GLY:CA	1:A:346:GLN:HE22	2.15	0.55
1:A:90:VAL:CA	1:A:293:MET:HE3	2.37	0.55
1:A:529:LYS:HZ3	1:A:538:THR:HG23	1.72	0.55
1:A:180:VAL:O	1:A:181:VAL:C	2.45	0.54
1:A:383:TYR:CE2	3:A:801:C8E:H42	2.41	0.54
1:A:164:THR:OG1	1:A:208:HIS:HD2	1.90	0.54
1:A:175:THR:OG1	1:A:175:THR:O	2.14	0.54
1:A:528:ASP:O	1:A:538:THR:HA	2.07	0.54
1:A:290:LEU:HD12	1:A:291:ASP:CA	2.37	0.54
1:A:146:SER:OG	1:A:586:TYR:N	2.35	0.54
1:A:6:ASP:HB2	1:A:106:ARG:HH22	1.72	0.54
1:A:120:SER:HB2	1:A:393:TYR:CZ	2.40	0.54
1:A:555:VAL:CG1	1:A:556:THR:HG23	2.16	0.54
1:A:528:ASP:CG	1:A:529:LYS:H	2.11	0.54
1:A:68:ILE:N	1:A:68:ILE:HD13	2.23	0.53
1:A:496:LEU:HD12	1:A:496:LEU:N	2.22	0.53
1:A:17:GLN:OE1	1:A:21:THR:HG22	2.07	0.53
1:A:164:THR:OG1	1:A:208:HIS:CD2	2.61	0.53
1:A:594:PHE:HD1	1:A:594:PHE:N	2.07	0.53
1:A:488:ASN:N	1:A:495:LEU:CD2	2.69	0.53
1:A:160:LEU:HD22	1:A:166:VAL:HG23	1.86	0.53
1:A:528:ASP:OD1	1:A:529:LYS:N	2.35	0.53
1:A:264:GLN:O	1:A:300:TRP:HD1	1.92	0.53
1:A:197:PHE:CE2	1:A:227:THR:HG21	2.44	0.53
1:A:176:HIS:HA	1:A:196:GLY:HA3	1.91	0.53
1:A:379:PHE:CE1	1:A:380:ILE:HD12	2.44	0.53
1:A:197:PHE:HA	1:A:227:THR:HA	1.91	0.53
1:A:502:GLN:OE1	1:A:523:LEU:CD2	2.57	0.53
1:A:138:THR:HB	1:A:156:THR:HB	1.89	0.53
1:A:380:ILE:O	1:A:381:GLU:C	2.44	0.52
1:A:198:LEU:HD13	1:A:198:LEU:C	2.30	0.52
1:A:592:TYR:C	1:A:592:TYR:CD1	2.83	0.52
1:A:293:MET:HE2	1:A:322:THR:HG22	1.92	0.52
1:A:567:ASN:HD21	1:A:571:LYS:H	1.56	0.52
1:A:75:HIS:CG	1:A:123:ILE:HD12	2.44	0.52
1:A:266:ILE:CG2	1:A:267:THR:N	2.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:N	1:A:278:ASP:OD2	2.41	0.52
1:A:120:SER:OG	1:A:121:ASP:OD1	2.20	0.52
1:A:77:LEU:HD11	1:A:79:LEU:HD23	1.90	0.52
1:A:178:TYR:O	1:A:179:ASP:CB	2.57	0.52
1:A:556:THR:OG1	1:A:558:HIS:N	2.33	0.52
1:A:379:PHE:O	1:A:380:ILE:CG1	2.51	0.52
1:A:18:PRO:O	1:A:21:THR:HB	2.09	0.52
1:A:174:HIS:HD2	1:A:174:HIS:C	2.08	0.51
1:A:212:ASP:O	1:A:213:ALA:CB	2.59	0.51
1:A:69:ARG:NH1	1:A:436:TYR:CD1	2.78	0.51
1:A:13:ASN:O	1:A:14:ARG:CB	2.53	0.51
1:A:257:ASN:CG	1:A:257:ASN:O	2.47	0.51
1:A:323:THR:CG2	1:A:324:PRO:N	2.74	0.51
1:A:426:THR:HG23	1:A:431:TRP:NE1	2.22	0.51
1:A:153:ASP:OD1	1:A:154:VAL:N	2.44	0.51
1:A:198:LEU:HD13	1:A:199:SER:N	2.25	0.51
1:A:111:ARG:NH2	1:A:465:GLU:OE2	2.43	0.51
1:A:165:ARG:CG	1:A:207:GLU:OE1	2.49	0.51
1:A:135:GLU:N	1:A:157:GLN:HE22	2.07	0.51
1:A:55:THR:HB	1:A:576:VAL:HG22	1.92	0.51
1:A:487:ARG:C	1:A:495:LEU:HD21	2.30	0.50
1:A:185:ASN:O	1:A:186:THR:CG2	2.59	0.50
1:A:534:TYR:CD1	1:A:535:PRO:CG	2.94	0.50
1:A:477:HIS:CE1	1:A:507:LEU:CD1	2.94	0.50
1:A:277:TYR:CG	1:A:278:ASP:HB3	2.46	0.50
1:A:526:ARG:CG	1:A:541:MET:CE	2.89	0.50
1:A:568:LEU:HD23	1:A:569:PHE:CE1	2.47	0.50
1:A:172:TYR:OH	1:A:174:HIS:ND1	2.27	0.50
1:A:531:TYR:C	1:A:533:SER:N	2.64	0.50
1:A:522:TYR:CD1	1:A:544:VAL:O	2.65	0.50
1:A:77:LEU:HG	1:A:79:LEU:CD2	2.41	0.50
1:A:333:TYR:CE1	1:A:402:TYR:CD1	3.00	0.49
1:A:592:TYR:CE1	1:A:594:PHE:HB3	2.47	0.49
1:A:514:PHE:CE2	1:A:553:TYR:CE1	3.00	0.49
1:A:47:ARG:HG2	1:A:48:ARG:N	2.10	0.49
1:A:404:PHE:CD2	1:A:404:PHE:O	2.48	0.49
1:A:534:TYR:CD1	1:A:535:PRO:N	2.81	0.49
1:A:90:VAL:HG22	1:A:293:MET:CE	2.41	0.49
1:A:289:THR:O	1:A:289:THR:OG1	2.29	0.49
1:A:134:ASP:OD1	1:A:134:ASP:C	2.51	0.49
1:A:116:ALA:HA	1:A:370:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:CD	1:A:541:MET:HE2	2.42	0.49
1:A:398:LEU:O	1:A:402:TYR:N	2.29	0.49
1:A:309:GLY:N	1:A:346:GLN:HE22	2.10	0.49
1:A:179:ASP:O	1:A:180:VAL:HG22	2.13	0.49
1:A:197:PHE:CD2	1:A:227:THR:HG21	2.47	0.49
1:A:185:ASN:OD1	1:A:185:ASN:N	2.32	0.49
1:A:13:ASN:HD22	1:A:14:ARG:N	2.11	0.49
1:A:226:ARG:HD2	1:A:244:LYS:HZ3	1.76	0.49
1:A:534:TYR:CE1	1:A:535:PRO:CB	2.96	0.49
1:A:278:ASP:OD1	1:A:279:PRO:CA	2.43	0.49
1:A:450:THR:OG1	1:A:452:LYS:HB2	2.13	0.49
1:A:516:TRP:CH2	1:A:551:VAL:HG11	2.48	0.49
1:A:162:ASP:CB	1:A:163:LYS:NZ	2.76	0.48
1:A:98:GLN:OE1	1:A:227:THR:HG21	2.13	0.48
1:A:516:TRP:CZ3	1:A:551:VAL:HG13	2.48	0.48
1:A:362:ASN:HD22	1:A:365:PHE:H	1.61	0.48
1:A:192:THR:CG2	1:A:192:THR:O	2.51	0.48
3:A:804:C8E:H112	3:A:804:C8E:H81	1.14	0.48
1:A:567:ASN:C	1:A:567:ASN:HD22	2.16	0.48
1:A:141:SER:O	1:A:142:ALA:HB2	2.14	0.48
1:A:397:ASN:C	1:A:397:ASN:OD1	2.52	0.48
1:A:351:PHE:CD1	1:A:351:PHE:N	2.82	0.48
1:A:169:LEU:HD13	1:A:170:GLY:C	2.34	0.48
1:A:534:TYR:CD1	1:A:535:PRO:CB	2.97	0.48
1:A:151:ASN:CG	1:A:152:TYR:N	2.67	0.48
1:A:185:ASN:ND2	1:A:579:TYR:OH	2.47	0.48
1:A:8:LEU:N	1:A:8:LEU:HD12	2.24	0.48
1:A:486:ALA:O	1:A:495:LEU:HG	2.14	0.47
1:A:510:GLN:CA	1:A:510:GLN:NE2	2.50	0.47
1:A:179:ASP:O	1:A:180:VAL:C	2.50	0.47
1:A:275:TYR:CD2	1:A:290:LEU:HB2	2.50	0.47
1:A:381:GLU:HG3	1:A:382:GLY:H	1.79	0.47
1:A:511:LEU:HG	1:A:512:TYR:CG	2.49	0.47
1:A:181:VAL:HG12	1:A:182:ALA:CA	2.33	0.47
1:A:469:ASN:ND2	1:A:469:ASN:N	2.61	0.47
1:A:244:LYS:NZ	1:A:246:TYR:CE2	2.83	0.47
1:A:555:VAL:HG12	1:A:556:THR:N	2.25	0.47
1:A:226:ARG:NH1	1:A:244:LYS:CD	2.72	0.47
1:A:529:LYS:HZ3	1:A:538:THR:CG2	2.28	0.47
1:A:516:TRP:CD2	1:A:551:VAL:CG1	2.97	0.47
1:A:266:ILE:HG22	1:A:267:THR:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TYR:CD2	1:A:229:TYR:N	2.82	0.47
1:A:217:PHE:O	1:A:252:ALA:HA	2.15	0.46
1:A:371:TRP:CE2	3:A:805:C8E:C6	2.97	0.46
1:A:278:ASP:CG	1:A:279:PRO:N	2.65	0.46
1:A:291:ASP:HB3	1:A:326:THR:HG23	1.96	0.46
3:A:803:C8E:H172	3:A:803:C8E:H112	1.97	0.46
1:A:87:LEU:HD11	1:A:223:TYR:OH	2.15	0.46
1:A:208:HIS:O	1:A:216:GLY:N	2.46	0.46
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.50	0.46
1:A:509:TRP:C	1:A:510:GLN:HE22	2.13	0.46
1:A:81:ASP:CG	1:A:219:ARG:HH12	2.19	0.46
1:A:19:ARG:C	1:A:21:THR:N	2.68	0.46
1:A:195:ASP:OD2	1:A:195:ASP:N	2.48	0.46
1:A:226:ARG:HH11	1:A:244:LYS:HG3	1.80	0.46
1:A:157:GLN:OE1	1:A:165:ARG:NH1	2.48	0.46
1:A:250:TRP:O	1:A:268:SER:OG	2.34	0.46
1:A:169:LEU:CD1	1:A:170:GLY:N	2.46	0.46
1:A:511:LEU:CD2	1:A:512:TYR:CE2	2.98	0.46
1:A:146:SER:HG	1:A:586:TYR:HB2	1.80	0.46
1:A:278:ASP:CB	1:A:280:HIS:O	2.63	0.46
1:A:473:GLY:C	1:A:475:LEU:H	2.19	0.46
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.29	0.46
1:A:245:LEU:C	1:A:245:LEU:HD22	2.36	0.45
1:A:321:THR:HA	1:A:333:TYR:O	2.16	0.45
1:A:450:THR:O	1:A:452:LYS:N	2.49	0.45
1:A:146:SER:O	1:A:147:ASN:CG	2.54	0.45
1:A:198:LEU:C	1:A:198:LEU:CD1	2.85	0.45
1:A:179:ASP:O	1:A:181:VAL:N	2.49	0.45
1:A:425:LEU:HD22	1:A:425:LEU:O	2.17	0.45
1:A:413:GLU:HG2	1:A:443:LEU:HA	1.97	0.45
1:A:450:THR:C	1:A:452:LYS:N	2.69	0.45
1:A:248:GLN:O	1:A:270:SER:HA	2.17	0.45
1:A:261:ILE:HA	1:A:304:VAL:HG12	1.97	0.45
1:A:99:PHE:HA	1:A:100:PRO:HD3	1.64	0.45
3:A:802:C8E:H31	3:A:802:C8E:H61	1.48	0.45
3:A:803:C8E:H172	3:A:803:C8E:C11	2.45	0.45
1:A:567:ASN:O	1:A:569:PHE:O	2.35	0.45
1:A:166:VAL:HG22	1:A:206:LEU:HD11	1.99	0.45
1:A:81:ASP:CB	1:A:219:ARG:HH12	2.30	0.45
1:A:516:TRP:CD2	1:A:551:VAL:HG12	2.51	0.45
1:A:126:VAL:HG13	1:A:127:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:CG	1:A:87:LEU:N	2.70	0.45
1:A:295:GLN:HG3	1:A:320:GLN:HG3	1.99	0.45
3:A:800:C8E:H101	3:A:800:C8E:H131	1.74	0.45
1:A:511:LEU:C	1:A:511:LEU:HD12	2.37	0.45
1:A:105:GLN:CA	1:A:105:GLN:NE2	2.79	0.45
1:A:296:TYR:N	1:A:319:LYS:O	2.36	0.44
1:A:385:PHE:C	1:A:385:PHE:CD2	2.88	0.44
1:A:362:ASN:HB3	1:A:365:PHE:CE2	2.52	0.44
1:A:81:ASP:CG	1:A:219:ARG:NH1	2.70	0.44
1:A:592:TYR:HD1	1:A:592:TYR:O	2.01	0.44
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.78	0.44
1:A:446:TYR:CE2	1:A:451:LEU:HA	2.53	0.44
3:A:803:C8E:H72	3:A:803:C8E:H101	1.09	0.44
1:A:471:ASP:OD1	1:A:476:THR:HG23	2.18	0.44
1:A:206:LEU:HA	1:A:206:LEU:HD12	1.78	0.44
1:A:592:TYR:CD1	1:A:592:TYR:O	2.70	0.44
1:A:502:GLN:OE1	1:A:523:LEU:HD21	2.18	0.44
1:A:181:VAL:O	1:A:182:ALA:HB2	2.17	0.44
1:A:397:ASN:O	1:A:398:LEU:C	2.57	0.44
1:A:174:HIS:O	1:A:174:HIS:CG	2.70	0.44
1:A:208:HIS:ND1	1:A:208:HIS:C	2.71	0.43
1:A:179:ASP:C	1:A:180:VAL:HG13	2.37	0.43
1:A:96:LEU:O	1:A:97:SER:C	2.56	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD12	1.13	0.43
3:A:802:C8E:C5	3:A:802:C8E:H13	2.45	0.43
1:A:509:TRP:CA	1:A:510:GLN:NE2	2.81	0.43
1:A:36:ARG:NH2	1:A:508:ASP:OD1	2.50	0.43
1:A:213:ALA:O	1:A:256:TYR:HA	2.17	0.43
1:A:116:ALA:HA	1:A:370:THR:HG22	2.00	0.43
1:A:62:GLN:O	1:A:63:LEU:C	2.54	0.43
1:A:446:TYR:CE1	1:A:448:ASP:HA	2.54	0.43
1:A:210:PHE:C	1:A:211:THR:HG23	2.39	0.43
1:A:138:THR:HA	1:A:155:SER:O	2.19	0.43
1:A:48:ARG:HH12	1:A:519:THR:HG21	1.83	0.43
1:A:193:ASP:O	1:A:195:ASP:OD2	2.35	0.43
1:A:98:GLN:NE2	1:A:225:ASN:CB	2.82	0.43
1:A:293:MET:HE2	1:A:293:MET:HB2	1.82	0.43
1:A:559:LEU:HD23	1:A:560:THR:N	2.34	0.43
1:A:98:GLN:HE22	1:A:225:ASN:CB	2.31	0.42
1:A:530:ASP:OD1	1:A:530:ASP:C	2.56	0.42
1:A:446:TYR:HH	1:A:451:LEU:CD1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:TRP:O	1:A:371:TRP:CG	2.72	0.42
1:A:275:TYR:CZ	1:A:290:LEU:HD22	2.52	0.42
1:A:543:GLY:C	1:A:544:VAL:HG13	2.40	0.42
1:A:369:GLY:HA3	3:A:800:C8E:C8	2.43	0.42
1:A:77:LEU:CD1	1:A:79:LEU:HD23	2.49	0.42
1:A:59:GLY:O	1:A:62:GLN:HG2	2.20	0.42
1:A:559:LEU:CD2	1:A:560:THR:N	2.83	0.42
1:A:142:ALA:HA	1:A:151:ASN:OD1	2.19	0.42
1:A:379:PHE:CD1	1:A:380:ILE:HD12	2.55	0.42
1:A:191:GLN:CB	1:A:230:ASP:OD2	2.64	0.42
1:A:226:ARG:HH11	1:A:244:LYS:CG	2.32	0.42
1:A:323:THR:HB	1:A:326:THR:OG1	2.19	0.42
1:A:334:ASP:OD2	1:A:336:ARG:NH2	2.33	0.42
3:A:804:C8E:H172	3:A:804:C8E:H201	1.49	0.42
1:A:371:TRP:O	1:A:391:THR:HB	2.20	0.41
1:A:397:ASN:CG	1:A:400:GLN:NE2	2.74	0.41
1:A:566:ALA:O	1:A:584:ARG:HA	2.21	0.41
1:A:370:THR:N	3:A:800:C8E:C8	2.82	0.41
1:A:77:LEU:CD1	1:A:79:LEU:CD2	2.98	0.41
1:A:523:LEU:HD23	1:A:523:LEU:HA	1.80	0.41
1:A:496:LEU:CD1	1:A:496:LEU:N	2.84	0.41
3:A:804:C8E:H71	3:A:804:C8E:H41	1.89	0.41
1:A:353:PHE:HB3	3:A:803:C8E:H191	2.02	0.41
1:A:553:TYR:HA	1:A:554:PRO:HD3	1.67	0.41
1:A:564:LYS:HG3	1:A:565:ILE:N	2.36	0.41
1:A:166:VAL:HG22	1:A:206:LEU:CD1	2.51	0.41
1:A:372:GLN:HA	1:A:390:GLY:HA2	2.03	0.41
1:A:263:SER:CB	1:A:302:ASN:ND2	2.83	0.41
1:A:407:ASN:HA	1:A:408:PRO:HD3	1.82	0.41
3:A:802:C8E:C17	3:A:802:C8E:C1	2.98	0.41
3:A:804:C8E:H171	3:A:804:C8E:H141	1.50	0.41
1:A:86:ASN:CG	1:A:87:LEU:H	2.25	0.41
1:A:358:ARG:HB3	1:A:370:THR:HG22	2.03	0.40
3:A:800:C8E:H81	3:A:800:C8E:H112	1.86	0.40
1:A:162:ASP:HB3	1:A:163:LYS:HZ2	1.87	0.40
1:A:351:PHE:HA	1:A:376:GLY:O	2.22	0.40
1:A:339:GLY:HA2	1:A:359:SER:O	2.21	0.40
1:A:49:LEU:O	1:A:504:LYS:NZ	2.54	0.40
1:A:107:VAL:HG12	1:A:108:GLU:N	2.36	0.40
1:A:162:ASP:OD1	1:A:162:ASP:N	2.54	0.40
1:A:290:LEU:HD12	1:A:291:ASP:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:C	1:A:451:LEU:CD2	2.88	0.40
1:A:447:ASP:CG	1:A:449:HIS:HB2	2.40	0.40
1:A:159:GLN:O	1:A:160:LEU:HD13	2.22	0.40
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.64	0.40
1:A:77:LEU:HD21	1:A:79:LEU:CD2	2.24	0.40
1:A:121:ASP:N	1:A:121:ASP:OD1	2.54	0.40
1:A:9:VAL:HG13	1:A:19:ARG:HG2	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	570/594 (96%)	499 (88%)	50 (9%)	21 (4%)	4	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	VAL
1	A	182	ALA
1	A	191	GLN
1	A	192	THR
1	A	278	ASP
1	A	287	SER
1	A	11	THR
1	A	147	ASN
1	A	176	HIS
1	A	184	GLY
1	A	186	THR
1	A	213	ALA
1	A	146	SER
1	A	178	TYR

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Mol	Chain	Res	Type
1	A	179	ASP
1	A	14	ARG
1	A	87	LEU
1	A	183	TYR
1	A	189	GLN
1	A	451	LEU
1	A	279	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	479/495 (97%)	396 (83%)	83 (17%)	2 11

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	VAL
1	A	13	ASN
1	A	21	THR
1	A	26	THR
1	A	47	ARG
1	A	60	SER
1	A	67	PHE
1	A	97	SER
1	A	103	LEU
1	A	114	ARG
1	A	121	ASP
1	A	138	THR
1	A	141	SER
1	A	148	SER
1	A	153	ASP
1	A	158	GLN
1	A	160	LEU
1	A	162	ASP

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Mol	Chain	Res	Type
1	A	169	LEU
1	A	172	TYR
1	A	174	HIS
1	A	175	THR
1	A	176	HIS
1	A	180	VAL
1	A	181	VAL
1	A	183	TYR
1	A	185	ASN
1	A	186	THR
1	A	189	GLN
1	A	195	ASP
1	A	198	LEU
1	A	200	LYS
1	A	207	GLU
1	A	215	SER
1	A	223	TYR
1	A	226	ARG
1	A	227	THR
1	A	229	TYR
1	A	242	THR
1	A	245	LEU
1	A	262	LYS
1	A	265	LEU
1	A	267	THR
1	A	272	SER
1	A	276	ASN
1	A	277	TYR
1	A	280	HIS
1	A	285	ASP
1	A	287	SER
1	A	290	LEU
1	A	345	LEU
1	A	346	GLN
1	A	348	VAL
1	A	367	ARG
1	A	370	THR
1	A	391	THR
1	A	398	LEU
1	A	404	PHE
1	A	407	ASN
1	A	414	LYS

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	426	THR
1	A	433	ILE
1	A	448	ASP
1	A	451	LEU
1	A	469	ASN
1	A	510	GLN
1	A	513	ASP
1	A	519	THR
1	A	526	ARG
1	A	533	SER
1	A	537	GLN
1	A	538	THR
1	A	557	SER
1	A	559	LEU
1	A	560	THR
1	A	567	ASN
1	A	568	LEU
1	A	571	LYS
1	A	572	ASP
1	A	591	SER
1	A	594	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	32	GLN
1	A	98	GLN
1	A	105	GLN
1	A	147	ASN
1	A	157	GLN
1	A	208	HIS
1	A	225	ASN
1	A	280	HIS
1	A	295	GLN
1	A	302	ASN
1	A	320	GLN
1	A	337	ASN
1	A	346	GLN
1	A	347	GLN
1	A	362	ASN

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	455	ASN
1	A	469	ASN
1	A	506	GLN
1	A	510	GLN
1	A	567	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	C8E	A	800	-	20,20,20	0.53	0	19,19,19	1.52	4 (21%)
3	C8E	A	801	-	20,20,20	0.48	0	19,19,19	0.61	0
3	C8E	A	802	-	20,20,20	0.41	0	19,19,19	1.35	1 (5%)
3	C8E	A	803	-	20,20,20	0.45	0	19,19,19	1.00	1 (5%)
3	C8E	A	804	-	20,20,20	0.46	0	19,19,19	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	C8E	A	805	-	20,20,20	0.57	0	19,19,19	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	800	-	-	0/18/18/18	0/0/0/0
3	C8E	A	801	-	-	0/18/18/18	0/0/0/0
3	C8E	A	802	-	-	0/18/18/18	0/0/0/0
3	C8E	A	803	-	-	0/18/18/18	0/0/0/0
3	C8E	A	804	-	-	0/18/18/18	0/0/0/0
3	C8E	A	805	-	-	0/18/18/18	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	C8E	O12-C13-C14	-3.11	96.53	110.36
3	A	800	C8E	O15-C14-C13	-3.09	96.65	110.36
3	A	802	C8E	C19-O18-C17	-2.74	101.54	113.31
3	A	800	C8E	O21-C20-C19	-2.37	97.42	112.03
3	A	800	C8E	C19-O18-C17	-2.25	103.62	113.31
3	A	803	C8E	O18-C19-C20	-2.20	100.31	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	C8E	12	0
3	A	801	C8E	1	0
3	A	802	C8E	7	0
3	A	803	C8E	6	0
3	A	804	C8E	4	0
3	A	805	C8E	7	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	576/594 (96%)	-0.26	16 (2%)	56	56	17, 30, 45, 61	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	532	SER	4.6
1	A	184	GLY	4.0
1	A	278	ASP	4.0
1	A	277	TYR	3.6
1	A	162	ASP	2.9
1	A	287	SER	2.8
1	A	242	THR	2.8
1	A	276	ASN	2.7
1	A	183	TYR	2.6
1	A	328	TYR	2.6
1	A	531	TYR	2.4
1	A	185	ASN	2.3
1	A	280	HIS	2.2
1	A	186	THR	2.2
1	A	190	ALA	2.2
1	A	163	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	C8E	A	804	21/21	0.77	0.35	7.19	48,69,82,88	0
3	C8E	A	805	21/21	0.72	0.46	5.09	48,86,117,120	0
3	C8E	A	801	21/21	0.84	0.34	4.50	45,76,99,107	0
3	C8E	A	803	21/21	0.83	0.29	3.13	55,79,97,103	0
3	C8E	A	802	21/21	0.94	0.23	1.84	39,58,75,77	0
3	C8E	A	800	21/21	0.91	0.19	0.12	51,66,75,83	0
2	CA	A	596	1/1	0.95	0.08	-1.67	94,94,94,94	0
2	CA	A	595	1/1	0.97	0.05	-2.28	78,78,78,78	0
2	CA	A	598	1/1	0.84	0.16	-	111,111,111,111	0
2	CA	A	597	1/1	0.66	0.12	-	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.