Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:54 PM JST

PDB ID	:	4TRW
Title	:	Structure of BACE1 complex with a syn-HEA-type inhibitor
Authors	:	Akaji, K.; Teruya, K.; Akiyama, T.; Sanjho, A.; Yamashita, E.; Nakagawa, A.
Deposited on	:	2014-06-18
Resolution	:	2.85 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:

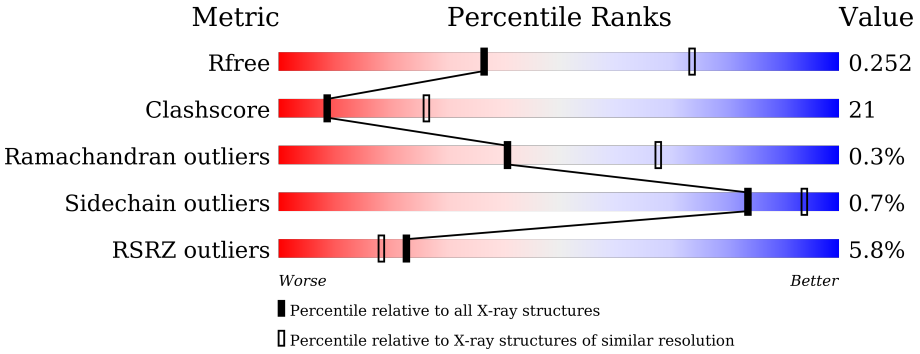
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	390	4% 75% 24%
1	B	390	5% 72% 27% •
1	C	390	8% 73% 25% •
2	D	4	75% 25%
2	E	4	50% 25% 25%
2	F	4	50% 25% 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9353 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3056	1957	507	578	14	0	0	0
1	B	389	3056	1957	507	578	14	0	0	0
1	C	390	3060	1959	508	579	14	0	0	0

- Molecule 2 is a protein called L-alpha-glutamyl-L-isoleucyl-N-[(2R,3S)-1-{[(1S)-1-carboxybutyl]amino}-2-hydroxy-5-methylhexan-3-yl]-3-thiophen-2-yl-L-alaninamide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	4	44	30	5	8	1	0	0	0
2	E	4	44	30	5	8	1	0	0	0
2	F	4	44	30	5	8	1	0	0	0

- Molecule 3 is water.

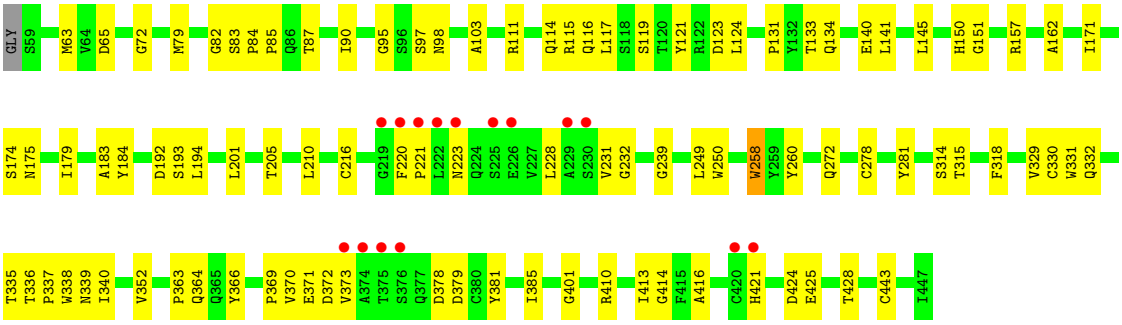
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	12	12	12	0	0
3	B	21	21	21	0	0
3	C	16	16	16	0	0

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.

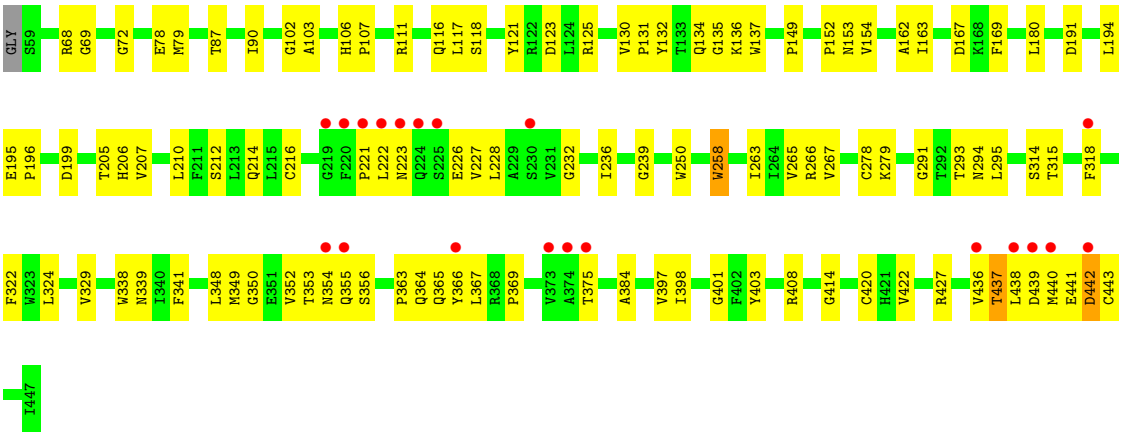
• Molecule 1: Beta-secretase 1

Chain A:



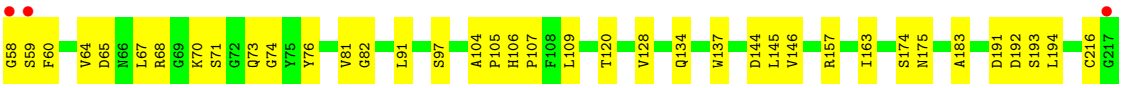
• Molecule 1: Beta-secretase 1

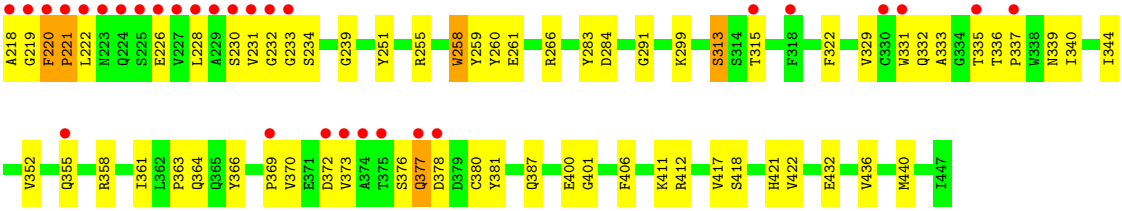
Chain B:



• Molecule 1: Beta-secretase 1

Chain C:





• Molecule 2: L-alpha-glutamyl-L-isoleucyl-N-[(2R,3S)-1-{[(1S)-1-carboxybutyl]amino}-2-hydroxy-5-methylhexan-3-yl]-3-thiophen-2-yl-L-alaninamide

Chain D:

• Molecule 2: L-alpha-glutamyl-L-isoleucyl-N-[(2R,3S)-1-{[(1S)-1-carboxybutyl]amino}-2-hydroxy-5-methylhexan-3-yl]-3-thiophen-2-yl-L-alaninamide

Chain E:

• Molecule 2: L-alpha-glutamyl-L-isoleucyl-N-[(2R,3S)-1-{[(1S)-1-carboxybutyl]amino}-2-hydroxy-5-methylhexan-3-yl]-3-thiophen-2-yl-L-alaninamide

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	82.28Å 103.66Å 102.00Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	49.72 – 2.85 49.72 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.72-2.85) 99.1 (49.72-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.208 , 0.238 0.207 , 0.252	Depositor DCC
R_{free} test set	1950 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.8	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	0.93	EDS
Total number of atoms	9353	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: TIH, LHE

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	0.61	0/3134	0.79	1/4262 (0.0%)
1	B	0.62	0/3134	0.81	1/4262 (0.0%)
1	C	0.59	0/3138	0.81	3/4267 (0.1%)
2	D	0.77	0/16	0.64	0/20
2	E	0.18	0/16	0.39	0/20
2	F	0.16	0/16	0.38	0/20
All	All	0.61	0/9454	0.80	5/12851 (0.0%)

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
2	D	0	1
2	E	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	220	PHE	C-N-CD	-13.29	91.37	120.60
1	B	191	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	234	SER	N-CA-C	5.21	125.08	111.00
1	A	98	ASN	N-CA-CB	-5.20	101.23	110.60
1	C	313	SER	CB-CA-C	-5.07	100.46	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	TIH	Peptide
2	E	3	TIH	Peptide
2	F	3	TIH	Peptide

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	3056	0	2969	92	0
1	B	3056	0	2969	155	0
1	C	3060	0	2970	141	0
2	D	44	0	39	5	0
2	E	44	0	39	6	0
2	F	44	0	39	5	0
3	A	12	0	0	2	0
3	B	21	0	0	1	0
3	C	16	0	0	1	0
All	All	9353	0	9025	374	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 21.

All (374) 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:C:219:GLY:HA3	1:C:220:PHE:CD2	1.42	1.55
1:B:363:PRO:HA	1:B:366:TYR:CE2	1.47	1.49
1:B:263:ILE:HG21	1:B:440:MET:CE	1.59	1.31
1:A:352:VAL:HG11	1:C:355:GLN:NE2	1.54	1.22
1:B:263:ILE:CG2	1:B:440:MET:HE2	1.69	1.22
1:A:338:TRP:CZ3	1:A:364:GLN:HA	1.77	1.18
1:C:369:PRO:HG3	1:C:381:TYR:CE1	1.79	1.16
1:B:436:VAL:HG21	1:C:436:VAL:CG2	1.78	1.14
1:C:219:GLY:HA3	1:C:220:PHE:CE2	1.82	1.14
1:B:265:VAL:HG21	1:B:437:THR:OG1	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:SER:HB3	1:B:437:THR:HG21	1.27	1.11
1:B:436:VAL:CG2	1:C:436:VAL:HG23	1.79	1.11
1:C:219:GLY:CA	1:C:220:PHE:CD2	2.33	1.10
1:C:331:TRP:HE3	1:C:336:THR:CG2	1.65	1.08
1:C:352:VAL:HB	1:C:355:GLN:OE1	1.53	1.08
1:C:219:GLY:HA3	1:C:220:PHE:CG	1.88	1.08
1:B:363:PRO:HB3	1:B:366:TYR:OH	1.54	1.08
1:C:331:TRP:HB2	1:C:336:THR:CG2	1.83	1.08
1:C:331:TRP:HB2	1:C:336:THR:HG22	1.11	1.08
1:B:263:ILE:CG2	1:B:440:MET:CE	2.25	1.07
1:B:363:PRO:CA	1:B:366:TYR:CE2	2.36	1.07
1:A:352:VAL:HG11	1:C:355:GLN:HE22	0.93	1.07
1:A:338:TRP:CH2	1:A:364:GLN:HA	1.91	1.05
1:B:356:SER:HB3	1:B:437:THR:CG2	1.85	1.05
1:B:132:TYR:HE2	1:B:137:TRP:NE1	1.54	1.04
1:B:263:ILE:HG21	1:B:440:MET:HE2	1.09	1.04
1:C:219:GLY:CA	1:C:220:PHE:CG	2.40	1.04
1:C:331:TRP:CE3	1:C:336:THR:CG2	2.40	1.03
1:B:356:SER:CB	1:B:437:THR:CG2	2.36	1.03
1:B:440:MET:HB3	1:B:441:GLU:HA	1.36	1.02
1:C:331:TRP:CB	1:C:336:THR:HG22	1.90	0.99
1:C:231:VAL:H	1:C:232:GLY:HA2	1.27	0.99
1:B:366:TYR:O	1:B:384:ALA:HB3	1.62	0.98
1:C:222:LEU:HD22	1:C:226:GLU:CD	1.84	0.97
1:B:356:SER:OG	1:B:437:THR:HG22	1.65	0.97
1:C:220:PHE:HB3	1:C:369:PRO:HB2	1.46	0.97
1:B:278:CYS:CB	1:B:443:CYS:SG	2.53	0.97
1:C:220:PHE:CB	1:C:369:PRO:HB2	1.95	0.96
1:C:331:TRP:CE3	1:C:336:THR:HB	2.01	0.96
1:B:436:VAL:HG21	1:C:436:VAL:HG23	0.96	0.95
1:B:356:SER:CB	1:B:437:THR:HG21	1.96	0.95
1:A:352:VAL:CG1	1:C:355:GLN:HE22	1.80	0.94
1:B:223:ASN:OD1	1:B:226:GLU:HB2	1.66	0.94
1:C:331:TRP:CE3	1:C:336:THR:HG22	2.03	0.94
1:B:265:VAL:HG12	1:B:440:MET:HE3	1.49	0.93
1:C:369:PRO:HG3	1:C:381:TYR:HE1	1.29	0.93
1:A:338:TRP:CZ3	1:A:364:GLN:CA	2.52	0.92
1:C:372:ASP:OD1	1:C:373:VAL:N	2.03	0.92
1:C:222:LEU:HD22	1:C:226:GLU:OE2	1.70	0.91
1:C:81:VAL:HG12	1:C:146:VAL:HG22	1.53	0.91
1:B:265:VAL:HG21	1:B:437:THR:CB	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:THR:HG23	1:B:437:THR:O	1.71	0.90
1:B:291:GLY:O	2:E:2:ILE:HD12	1.71	0.89
1:C:417:VAL:HG13	1:C:421:HIS:NE2	1.88	0.89
1:A:364:GLN:NE2	1:A:424:ASP:HB2	1.89	0.88
1:B:349:MET:SD	1:B:440:MET:SD	2.72	0.88
1:C:369:PRO:HG3	1:C:381:TYR:CD1	2.09	0.88
1:B:278:CYS:HB2	1:B:443:CYS:SG	2.14	0.88
1:B:279:LYS:HG2	1:B:442:ASP:O	1.72	0.87
1:B:439:ASP:OD2	1:C:266:ARG:HD2	1.74	0.87
1:B:363:PRO:HA	1:B:366:TYR:CZ	2.08	0.87
1:B:265:VAL:CG2	1:B:437:THR:OG1	2.22	0.86
1:C:331:TRP:CE3	1:C:336:THR:CB	2.58	0.86
1:B:436:VAL:CG2	1:C:436:VAL:CG2	2.46	0.86
1:C:231:VAL:N	1:C:232:GLY:HA2	1.83	0.85
1:B:265:VAL:CG1	1:B:440:MET:HE3	2.08	0.84
1:C:67:LEU:HB2	1:C:233:GLY:O	1.78	0.83
1:B:294:ASN:HB3	1:B:384:ALA:O	1.77	0.83
1:B:440:MET:CB	1:B:441:GLU:HA	2.05	0.82
1:B:356:SER:CB	1:B:437:THR:HG22	2.08	0.82
1:B:263:ILE:CG2	1:B:440:MET:HE1	2.10	0.82
1:B:366:TYR:CE1	1:B:367:LEU:HG	2.15	0.81
1:B:222:LEU:HD12	1:B:222:LEU:O	1.80	0.81
1:B:356:SER:OG	1:B:437:THR:CG2	2.26	0.81
1:C:331:TRP:HE3	1:C:336:THR:HG21	1.47	0.80
1:C:355:GLN:O	1:C:440:MET:SD	2.40	0.80
1:C:231:VAL:HB	1:C:233:GLY:N	1.97	0.80
1:B:265:VAL:HG11	1:B:437:THR:OG1	1.81	0.80
1:C:220:PHE:CD2	1:C:369:PRO:HG2	2.17	0.79
1:B:440:MET:HA	1:B:442:ASP:H	1.47	0.78
1:A:318:PHE:HD1	1:A:329:VAL:HG11	1.47	0.78
1:B:366:TYR:O	1:B:384:ALA:CB	2.32	0.78
1:C:230:SER:OG	1:C:231:VAL:HG22	1.84	0.77
1:C:222:LEU:CD2	1:C:226:GLU:OE2	2.32	0.77
1:B:265:VAL:HG11	1:B:437:THR:HG1	1.50	0.76
1:C:331:TRP:CD2	1:C:336:THR:HG22	2.22	0.75
1:C:106:HIS:CG	1:C:107:PRO:HD2	2.22	0.75
1:C:219:GLY:HA2	1:C:220:PHE:CG	2.20	0.75
1:C:258:TRP:HD1	1:C:258:TRP:H	1.33	0.75
1:B:294:ASN:CB	1:B:384:ALA:O	2.34	0.75
1:B:136:LYS:HD2	1:B:167:ASP:HB3	1.70	0.74
1:C:331:TRP:CG	1:C:336:THR:HG22	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TYR:CE2	1:B:137:TRP:NE1	2.40	0.73
1:B:263:ILE:HG22	1:B:440:MET:HE2	1.69	0.73
1:B:132:TYR:HE2	1:B:137:TRP:HE1	0.80	0.73
1:B:440:MET:HB3	1:B:441:GLU:CA	2.16	0.73
1:C:68:ARG:HG2	1:C:230:SER:O	1.88	0.73
1:A:221:PRO:CG	1:A:371:GLU:HG2	2.18	0.72
1:C:144:ASP:OD1	1:C:145:LEU:N	2.22	0.72
1:B:279:LYS:CG	1:B:442:ASP:O	2.37	0.71
1:C:332:GLN:HB2	1:C:335:THR:OG1	1.90	0.71
1:A:221:PRO:HG3	1:A:371:GLU:HG2	1.72	0.71
1:C:315:THR:HG23	3:C:615:HOH:O	1.91	0.69
1:B:439:ASP:O	1:B:440:MET:HB2	1.93	0.69
1:B:136:LYS:HB2	1:B:167:ASP:O	1.92	0.69
1:B:278:CYS:SG	1:B:438:LEU:HD23	2.32	0.69
1:B:365:GLN:O	1:B:397:VAL:HB	1.92	0.69
1:B:265:VAL:HG12	1:B:440:MET:CE	2.22	0.69
1:B:350:GLY:H	1:B:356:SER:HB3	1.56	0.68
1:B:353:THR:CG2	1:B:437:THR:O	2.40	0.68
1:C:291:GLY:O	2:F:2:ILE:HG13	1.93	0.68
1:B:363:PRO:HA	1:B:366:TYR:HE2	1.49	0.68
1:A:192:ASP:O	1:A:194:LEU:N	2.27	0.68
1:B:263:ILE:HG22	1:B:440:MET:CE	2.21	0.68
1:A:364:GLN:HE22	1:A:424:ASP:HB2	1.58	0.68
1:B:363:PRO:HA	1:B:366:TYR:CD2	2.24	0.67
1:C:417:VAL:CG1	1:C:421:HIS:NE2	2.58	0.67
1:A:220:PHE:O	1:A:221:PRO:C	2.33	0.67
1:C:219:GLY:HA2	1:C:220:PHE:CD1	2.30	0.67
1:C:220:PHE:CB	1:C:369:PRO:CB	2.72	0.66
1:B:130:VAL:HB	1:B:137:TRP:CZ2	2.31	0.66
1:C:377:GLN:HE21	1:C:377:GLN:HA	1.61	0.65
1:A:221:PRO:HB2	1:A:371:GLU:HG3	1.77	0.65
1:C:377:GLN:HA	1:C:377:GLN:NE2	2.09	0.65
1:B:322:PHE:CD1	1:B:329:VAL:HG13	2.31	0.65
1:B:341:PHE:HB3	1:B:366:TYR:OH	1.97	0.65
1:A:338:TRP:HZ3	1:A:364:GLN:CA	2.08	0.65
1:B:136:LYS:CB	1:B:167:ASP:HB3	2.27	0.64
1:B:352:VAL:HG12	1:B:354:ASN:H	1.62	0.64
1:B:265:VAL:CG1	1:B:440:MET:CE	2.76	0.64
1:A:272:GLN:HE22	1:B:427:ARG:HD2	1.61	0.64
1:B:199:ASP:OD1	1:B:408:ARG:NH2	2.31	0.64
1:C:106:HIS:ND1	1:C:107:PRO:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:VAL:CG1	1:B:437:THR:OG1	2.47	0.62
1:B:279:LYS:NZ	1:B:442:ASP:O	2.24	0.62
1:A:314:SER:HB2	1:B:339:ASN:ND2	2.15	0.62
1:B:265:VAL:CB	1:B:437:THR:OG1	2.47	0.62
1:B:134:GLN:HG3	1:B:134:GLN:O	2.00	0.62
1:C:67:LEU:HB2	1:C:233:GLY:C	2.21	0.61
1:B:294:ASN:CG	1:B:384:ALA:O	2.39	0.61
1:A:72:GLY:O	2:D:1:GLU:N	2.28	0.61
1:C:220:PHE:CG	1:C:369:PRO:HG2	2.35	0.61
1:A:338:TRP:HZ3	1:A:363:PRO:C	2.03	0.61
1:C:220:PHE:HB2	1:C:369:PRO:CB	2.31	0.61
1:A:82:GLY:O	1:A:85:PRO:HA	2.00	0.61
1:B:152:PRO:O	1:B:154:VAL:HG22	1.99	0.61
1:B:263:ILE:HG21	1:B:440:MET:SD	2.40	0.60
1:C:219:GLY:CA	1:C:220:PHE:CD1	2.85	0.60
1:A:331:TRP:O	1:A:378:ASP:HB2	2.01	0.60
1:B:338:TRP:HZ3	1:B:367:LEU:HD12	1.65	0.60
1:C:344:ILE:HB	1:C:361:ILE:HG22	1.82	0.60
1:C:339:ASN:OD1	1:C:340:ILE:N	2.35	0.60
1:B:136:LYS:HB2	1:B:167:ASP:HB3	1.83	0.60
1:C:230:SER:OG	1:C:231:VAL:CG2	2.49	0.60
1:B:363:PRO:HB3	1:B:366:TYR:CZ	2.37	0.59
1:A:338:TRP:CZ3	1:A:364:GLN:N	2.70	0.59
1:C:220:PHE:HB2	1:C:369:PRO:HB2	1.83	0.59
1:A:338:TRP:HZ3	1:A:364:GLN:N	2.01	0.59
1:B:214:GLN:NE2	1:B:420:CYS:SG	2.75	0.59
1:C:222:LEU:CD2	1:C:226:GLU:CD	2.67	0.59
1:A:338:TRP:HZ3	1:A:364:GLN:HA	1.56	0.58
1:B:375:THR:O	1:B:375:THR:HG22	2.03	0.58
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.39	0.58
1:B:265:VAL:HG21	1:B:437:THR:HB	1.83	0.58
1:A:401:GLY:HA2	1:A:421:HIS:ND1	2.19	0.58
1:A:123:ASP:OD1	1:A:124:LEU:N	2.36	0.57
1:C:221:PRO:HG2	1:C:370:VAL:C	2.24	0.57
1:B:363:PRO:CA	1:B:366:TYR:CZ	2.80	0.56
1:C:231:VAL:HB	1:C:233:GLY:H	1.70	0.56
1:A:103:ALA:CB	1:A:162:ALA:HB1	2.36	0.56
1:C:258:TRP:CG	1:C:259:TYR:N	2.73	0.56
1:A:63:MET:HG2	1:A:150:HIS:O	2.06	0.55
1:A:192:ASP:O	1:A:193:SER:C	2.44	0.55
1:C:134:GLN:OE1	2:F:3:TIH:HD	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ASP:O	1:C:193:SER:C	2.44	0.55
1:B:210:LEU:HD11	1:B:239:GLY:HA2	1.88	0.55
1:C:71:SER:HB3	1:C:400:GLU:OE1	2.07	0.55
1:A:221:PRO:HB2	1:A:371:GLU:CG	2.36	0.55
1:B:363:PRO:CA	1:B:366:TYR:HE2	2.10	0.54
1:A:83:SER:O	1:A:119:SER:N	2.36	0.54
1:A:332:GLN:HB3	1:A:335:THR:OG1	2.08	0.54
1:C:216:CYS:HB2	1:C:231:VAL:HG11	1.89	0.54
1:B:363:PRO:CB	1:B:366:TYR:OH	2.43	0.54
1:A:339:ASN:ND2	1:B:314:SER:HB2	2.23	0.54
1:B:102:GLY:HA2	1:B:163:ILE:HB	1.89	0.54
1:C:128:VAL:HG13	1:C:137:TRP:HZ3	1.73	0.54
1:B:350:GLY:HA3	1:B:355:GLN:HB2	1.90	0.54
1:B:291:GLY:C	2:E:2:ILE:HD12	2.27	0.53
1:C:418:SER:HB3	1:C:421:HIS:HD2	1.72	0.53
1:A:201:LEU:O	1:A:205:THR:OG1	2.20	0.53
1:C:231:VAL:HB	1:C:232:GLY:C	2.27	0.53
1:C:70:LYS:HE2	1:C:73:GLN:HG3	1.91	0.53
1:A:115:ARG:NH2	1:A:140:GLU:OE2	2.41	0.53
1:B:87:THR:HG22	1:B:111:ARG:HH12	1.74	0.53
1:A:87:THR:HG22	1:A:111:ARG:HH12	1.73	0.52
1:C:67:LEU:N	1:C:233:GLY:O	2.42	0.52
1:C:258:TRP:CD1	1:C:258:TRP:N	2.71	0.52
1:C:372:ASP:CG	1:C:373:VAL:N	2.62	0.52
1:C:175:ASN:ND2	1:C:228:LEU:HD23	2.24	0.52
1:B:130:VAL:HB	1:B:137:TRP:CE2	2.44	0.52
1:B:436:VAL:HG22	1:C:436:VAL:CG2	2.38	0.52
1:C:259:TYR:CE1	2:F:4:LHE:O	2.62	0.52
1:C:332:GLN:O	1:C:335:THR:N	2.35	0.52
1:C:369:PRO:CG	1:C:381:TYR:CD1	2.89	0.52
1:B:205:THR:HG22	1:B:206:HIS:N	2.24	0.51
1:A:175:ASN:HD21	1:A:228:LEU:HD21	1.75	0.51
1:B:136:LYS:HD2	1:B:167:ASP:CB	2.39	0.51
1:C:219:GLY:CA	1:C:220:PHE:CE2	2.74	0.51
1:A:278:CYS:CB	1:A:443:CYS:HG	2.23	0.51
1:C:332:GLN:O	1:C:335:THR:CB	2.58	0.51
1:C:97:SER:OG	1:C:183:ALA:O	2.29	0.51
1:B:363:PRO:CB	1:B:366:TYR:CZ	2.94	0.51
1:B:130:VAL:CG2	1:B:137:TRP:CH2	2.94	0.50
1:B:352:VAL:H	1:B:355:GLN:HB2	1.76	0.50
1:B:356:SER:OG	1:B:437:THR:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:CYS:CB	1:A:443:CYS:SG	3.00	0.50
1:B:79:MET:SD	1:B:90:ILE:HG13	2.51	0.50
1:B:153:ASN:O	1:B:154:VAL:HG13	2.11	0.50
1:C:174:SER:O	1:C:175:ASN:CB	2.58	0.50
1:B:212:SER:HB3	1:B:403:TYR:CE1	2.46	0.50
1:B:439:ASP:OD2	1:C:266:ARG:CD	2.54	0.50
1:C:401:GLY:O	1:C:421:HIS:CD2	2.65	0.50
1:A:278:CYS:HG	1:A:443:CYS:HG	1.45	0.50
1:B:169:PHE:CE1	2:E:4:LHE:H33	2.47	0.49
1:C:106:HIS:CG	1:C:107:PRO:CD	2.93	0.49
1:B:440:MET:HA	1:B:442:ASP:N	2.22	0.49
1:C:418:SER:O	1:C:421:HIS:CD2	2.65	0.49
1:C:218:ALA:HA	1:C:422:VAL:HG23	1.93	0.49
1:C:372:ASP:OD1	1:C:373:VAL:HG12	2.13	0.49
1:C:418:SER:HB3	1:C:421:HIS:CD2	2.46	0.49
1:B:68:ARG:HD2	1:B:228:LEU:HA	1.94	0.49
1:C:332:GLN:O	1:C:333:ALA:C	2.48	0.49
1:C:192:ASP:O	1:C:194:LEU:N	2.45	0.49
1:C:331:TRP:CZ3	1:C:336:THR:HB	2.47	0.49
1:A:221:PRO:CB	1:A:371:GLU:HG2	2.43	0.49
1:C:64:VAL:O	1:C:65:ASP:HB2	2.12	0.49
1:C:67:LEU:CB	1:C:233:GLY:O	2.57	0.49
1:B:295:LEU:HB2	1:B:398:ILE:HD11	1.94	0.48
1:B:364:GLN:HG2	1:B:422:VAL:HG11	1.96	0.48
1:A:318:PHE:CD1	1:A:329:VAL:HG11	2.38	0.48
1:A:339:ASN:HD21	1:B:314:SER:HB2	1.78	0.48
1:A:401:GLY:HA2	1:A:421:HIS:HD1	1.78	0.48
1:C:82:GLY:HA2	1:C:144:ASP:OD2	2.12	0.48
1:C:329:VAL:O	1:C:380:CYS:HA	2.13	0.48
1:C:299:LYS:HG3	1:C:387:GLN:OE1	2.14	0.48
1:B:258:TRP:HD1	1:B:258:TRP:H	1.59	0.48
1:C:251:TYR:CD1	1:C:412:ARG:HG3	2.48	0.48
1:A:216:CYS:N	1:A:232:GLY:O	2.41	0.48
1:B:222:LEU:HD13	1:B:227:VAL:HG22	1.95	0.48
1:A:124:LEU:HD12	1:A:141:LEU:HB3	1.95	0.48
1:A:179:ILE:O	1:A:179:ILE:HG23	2.13	0.48
1:A:369:PRO:O	1:A:370:VAL:CG1	2.61	0.48
1:B:348:LEU:O	1:B:356:SER:HB2	2.14	0.48
1:B:90:ILE:HG21	1:B:180:LEU:HB2	1.96	0.47
1:B:250:TRP:O	1:B:414:GLY:HA2	2.14	0.47
1:C:74:GLY:HA3	1:C:91:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TYR:OH	1:C:175:ASN:ND2	2.23	0.47
1:C:106:HIS:CD2	1:C:107:PRO:HD2	2.49	0.47
1:A:337:PRO:O	1:A:340:ILE:HG12	2.15	0.47
1:B:436:VAL:O	1:B:436:VAL:HG13	2.13	0.47
1:B:194:LEU:O	1:B:195:GLU:C	2.53	0.47
1:B:366:TYR:CE1	1:B:367:LEU:CG	2.93	0.47
1:A:330:CYS:HA	1:A:379:ASP:O	2.14	0.47
1:A:260:TYR:HB3	1:A:413:ILE:HD11	1.95	0.47
1:A:332:GLN:HA	1:A:378:ASP:HB2	1.97	0.46
1:A:223:ASN:OD1	1:A:371:GLU:OE2	2.33	0.46
1:B:123:ASP:OD1	1:B:125:ARG:N	2.33	0.46
1:C:231:VAL:HB	1:C:232:GLY:CA	2.46	0.46
1:C:60:PHE:CZ	1:C:239:GLY:HA3	2.51	0.46
1:A:63:MET:HG2	1:A:151:GLY:HA2	1.98	0.46
1:C:364:GLN:OE1	1:C:364:GLN:N	2.41	0.46
1:B:365:GLN:NE2	1:B:401:GLY:HA3	2.31	0.46
1:C:106:HIS:HB3	1:C:109:LEU:HG	1.97	0.46
1:A:84:PRO:HA	1:A:85:PRO:HD3	1.78	0.46
1:A:210:LEU:HD11	1:A:239:GLY:HA2	1.97	0.46
1:A:424:ASP:OD1	1:A:425:GLU:N	2.49	0.46
1:B:106:HIS:O	1:B:107:PRO:C	2.54	0.46
1:C:363:PRO:HA	1:C:366:TYR:CD2	2.51	0.46
1:A:117:LEU:HD12	1:A:117:LEU:N	2.31	0.45
1:A:192:ASP:C	1:A:194:LEU:N	2.64	0.45
1:A:331:TRP:HB2	1:A:336:THR:HG22	1.97	0.45
1:B:279:LYS:HA	1:B:443:CYS:O	2.17	0.45
2:E:3:TIH:CD	2:E:3:TIH:N	2.79	0.45
1:B:354:ASN:ND2	3:B:621:HOH:O	2.50	0.45
1:A:314:SER:O	1:A:315:THR:C	2.55	0.45
1:B:130:VAL:CG2	1:B:137:TRP:CZ2	2.99	0.45
1:C:65:ASP:HA	1:C:232:GLY:O	2.16	0.45
1:A:410:ARG:CD	3:A:612:HOH:O	2.64	0.45
1:C:283:TYR:HA	1:C:284:ASP:HA	1.81	0.45
1:C:120:THR:HB	1:C:157:ARG:HH22	1.82	0.45
1:A:115:ARG:HH11	1:A:162:ALA:CB	2.30	0.45
1:A:192:ASP:C	1:A:194:LEU:H	2.20	0.45
1:A:336:THR:HG21	1:A:381:TYR:CE1	2.52	0.45
1:A:95:GLY:O	2:D:4:LHE:H49	2.17	0.45
1:C:322:PHE:CD1	1:C:329:VAL:HG23	2.51	0.45
1:C:137:TRP:HB2	1:C:163:ILE:HG23	1.99	0.45
1:C:255:ARG:HD3	1:C:261:GLU:OE2	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:HH11	1:A:162:ALA:HB1	1.82	0.44
1:B:436:VAL:CG2	1:C:436:VAL:HG21	2.40	0.44
1:A:221:PRO:CB	1:A:371:GLU:CG	2.95	0.44
1:C:97:SER:OG	1:C:183:ALA:C	2.56	0.44
1:A:410:ARG:HD3	3:A:612:HOH:O	2.17	0.44
1:C:191:ASP:O	1:C:192:ASP:C	2.56	0.44
2:F:1:GLU:OE2	2:F:3:TIH:HE2	2.18	0.44
1:B:216:CYS:HB2	1:B:232:GLY:O	2.18	0.44
1:A:278:CYS:O	1:A:281:TYR:N	2.42	0.44
1:B:375:THR:O	1:B:375:THR:CG2	2.64	0.44
1:C:260:TYR:CE1	1:C:406:PHE:HD2	2.35	0.44
1:A:192:ASP:OD1	1:A:193:SER:N	2.51	0.44
1:B:205:THR:HG21	1:B:207:VAL:HG23	1.99	0.43
1:C:313:SER:HA	1:C:340:ILE:HG12	2.00	0.43
1:C:411:LYS:HE2	1:C:411:LYS:HB3	1.94	0.43
1:A:372:ASP:OD1	1:A:373:VAL:N	2.52	0.43
1:C:230:SER:HA	1:C:231:VAL:HA	1.72	0.43
1:A:133:THR:HB	2:D:3:TIH:HB2	2.00	0.43
1:B:356:SER:OG	1:B:437:THR:HB	2.18	0.43
1:C:70:LYS:CE	1:C:73:GLN:HG3	2.48	0.43
1:A:65:ASP:CG	1:A:231:VAL:HG11	2.39	0.43
1:B:293:THR:OG1	2:E:2:ILE:HG13	2.19	0.43
1:A:134:GLN:HB3	2:D:3:TIH:HB3	2.00	0.43
1:A:174:SER:O	1:A:175:ASN:CB	2.66	0.43
1:A:97:SER:OG	1:A:184:TYR:O	2.34	0.43
1:A:115:ARG:HD2	1:A:121:TYR:CZ	2.54	0.43
1:A:336:THR:HG21	1:A:381:TYR:HE1	1.83	0.43
1:A:338:TRP:CH2	1:A:364:GLN:HG3	2.54	0.43
1:B:266:ARG:HG2	1:B:267:VAL:N	2.34	0.43
1:B:350:GLY:HA3	1:B:355:GLN:CB	2.49	0.43
1:C:329:VAL:HG11	1:C:331:TRP:CZ2	2.54	0.43
1:B:103:ALA:CB	1:B:162:ALA:HB1	2.49	0.42
1:C:58:GLY:O	1:C:59:SER:OG	2.25	0.42
1:A:183:ALA:HA	1:A:260:TYR:CE2	2.54	0.42
1:A:258:TRP:HD1	1:A:258:TRP:H	1.66	0.42
1:A:428:THR:O	1:A:428:THR:HG23	2.18	0.42
1:B:214:GLN:CD	1:B:420:CYS:SG	2.98	0.42
1:C:358:ARG:NH2	1:C:432:GLU:OE2	2.52	0.42
1:C:376:SER:O	1:C:378:ASP:N	2.49	0.42
1:B:366:TYR:CD1	1:B:367:LEU:HG	2.51	0.42
1:C:344:ILE:HB	1:C:361:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:SER:HB3	1:B:121:TYR:HB2	2.01	0.42
1:B:212:SER:HB2	1:B:236:ILE:HB	2.01	0.42
1:C:218:ALA:HA	1:C:422:VAL:CG2	2.50	0.42
1:B:69:GLY:HA2	1:B:227:VAL:HG13	2.01	0.42
1:B:132:TYR:HE2	1:B:137:TRP:CD1	2.30	0.42
1:C:222:LEU:HD23	1:C:226:GLU:OE2	2.18	0.42
1:B:314:SER:O	1:B:315:THR:C	2.57	0.42
1:A:79:MET:SD	1:A:90:ILE:HG13	2.60	0.41
1:B:130:VAL:HG23	1:B:137:TRP:CH2	2.55	0.41
1:B:221:PRO:HG3	1:B:369:PRO:HB2	2.01	0.41
1:B:222:LEU:CD1	1:B:227:VAL:HG22	2.50	0.41
1:C:104:ALA:HB1	1:C:105:PRO:HD2	2.01	0.41
1:A:171:ILE:HD11	2:D:2:ILE:HG22	2.03	0.41
1:A:250:TRP:O	1:A:414:GLY:HA2	2.19	0.41
1:B:72:GLY:O	2:E:1:GLU:N	2.40	0.41
1:B:278:CYS:O	1:B:279:LYS:C	2.59	0.41
1:A:249:LEU:HD23	1:A:416:ALA:HB2	2.02	0.41
1:B:258:TRP:CD1	1:B:258:TRP:N	2.89	0.41
1:C:82:GLY:CA	1:C:144:ASP:OD2	2.69	0.41
1:A:314:SER:HB2	1:B:339:ASN:HD22	1.85	0.41
1:B:116:GLN:HG2	1:B:117:LEU:HD12	2.02	0.41
1:B:195:GLU:HA	1:B:196:PRO:HD3	1.93	0.41
1:C:220:PHE:CG	1:C:369:PRO:CG	3.03	0.41
1:B:338:TRP:CZ3	1:B:367:LEU:HD12	2.52	0.41
1:B:350:GLY:HA3	1:B:356:SER:N	2.36	0.41
1:A:114:GLN:OE1	1:A:117:LEU:HD22	2.21	0.40
1:A:116:GLN:HG2	1:A:117:LEU:HD12	2.01	0.40
1:C:258:TRP:HE1	1:C:261:GLU:HB2	1.87	0.40
1:A:366:TYR:HB2	1:A:385:ILE:HG13	2.04	0.40
1:B:78:GLU:O	1:B:149:PRO:HD2	2.22	0.40
1:B:318:PHE:HD1	1:B:329:VAL:HG11	1.84	0.40
1:A:145:LEU:HD23	1:A:157:ARG:HB2	2.02	0.40
1:B:132:TYR:HB2	1:B:135:GLY:HA3	2.02	0.40
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.98	0.40
1:C:291:GLY:O	2:F:2:ILE:CG1	2.67	0.40
1:C:418:SER:CB	1:C:421:HIS:HD2	2.34	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	387/390 (99%)	381 (98%)	5 (1%)	1 (0%)	41	68
1	B	387/390 (99%)	379 (98%)	7 (2%)	1 (0%)	41	68
1	C	388/390 (100%)	379 (98%)	7 (2%)	2 (0%)	29	57
2	D	1/4 (25%)	1 (100%)	0	0	100	100
2	E	1/4 (25%)	1 (100%)	0	0	100	100
2	F	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1165/1182 (99%)	1142 (98%)	19 (2%)	4 (0%)	41	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	PRO
1	C	337	PRO
1	A	131	PRO
1	B	131	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	332/332 (100%)	331 (100%)	1 (0%)	92	97
1	B	332/332 (100%)	329 (99%)	3 (1%)	78	92
1	C	332/332 (100%)	330 (99%)	2 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	2/2 (100%)	2 (100%)	0	100 100
2	E	2/2 (100%)	1 (50%)	1 (50%)	0 0
2	F	2/2 (100%)	2 (100%)	0	100 100
All	All	1002/1002 (100%)	995 (99%)	7 (1%)	84 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	TRP
1	B	258	TRP
1	B	437	THR
1	B	442	ASP
1	C	258	TRP
1	C	377	GLN
2	E	2	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	224	GLN
1	A	272	GLN
1	A	365	GLN
1	B	134	GLN
1	B	214	GLN
1	B	354	ASN
1	C	175	ASN
1	C	377	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	LHE	D	4	2	16,16,16	1.00	0	14,20,20	1.13	0
2	LHE	E	4	2	16,16,16	0.87	0	14,20,20	1.25	0
2	LHE	F	4	2	16,16,16	1.09	1 (6%)	14,20,20	1.60	2 (14%)
2	TIH	E	3	2	9,10,11	1.98	4 (44%)	3,12,14	2.90	2 (66%)
2	TIH	D	3	2	9,10,11	1.96	2 (22%)	3,12,14	4.13	1 (33%)
2	TIH	F	3	2	9,10,11	4.98	2 (22%)	3,12,14	3.68	1 (33%)

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	LHE	D	4	2	-	10/20/20/20	-
2	LHE	E	4	2	-	11/20/20/20	-
2	LHE	F	4	2	-	4/20/20/20	-
2	TIH	E	3	2	-	2/4/6/8	0/1/1/1
2	TIH	D	3	2	-	1/4/6/8	0/1/1/1
2	TIH	F	3	2	-	0/4/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	TIH	CB-CG	13.73	1.57	1.50
2	F	3	TIH	CG-SD	-5.30	1.62	1.73
2	D	3	TIH	CB-CG	4.51	1.52	1.50
2	E	3	TIH	CB-CG	-3.10	1.49	1.50
2	E	3	TIH	CG-SD	2.84	1.79	1.73
2	D	3	TIH	CG-SD	-2.81	1.67	1.73
2	E	3	TIH	CD-CG	-2.57	1.31	1.37
2	E	3	TIH	CB-CA	-2.48	1.48	1.53
2	F	4	LHE	C21-CA2	-2.12	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	TIH	CE1-CE2-SD	-6.92	107.36	112.98
2	F	3	TIH	CE1-CE2-SD	-6.35	107.83	112.98
2	E	3	TIH	CE1-CE2-SD	-4.05	109.70	112.98
2	F	4	LHE	C25-C20-N5	3.22	120.24	112.00
2	F	4	LHE	C22-C21-CA2	-3.08	109.20	115.82
2	E	3	TIH	CB-CA-C	-2.65	106.51	111.47

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	LHE	C22-C21-CA2-N
2	D	4	LHE	N5-C20-C25-CA2
2	D	4	LHE	N5-C20-C25-O6
2	D	4	LHE	C27-CA-N5-C20
2	E	4	LHE	C22-C21-CA2-C25
2	E	4	LHE	N5-C20-C25-CA2
2	E	4	LHE	N5-C20-C25-O6
2	E	4	LHE	C28-C27-CA-N5
2	F	4	LHE	C-CA-N5-C20
2	E	4	LHE	CA-C27-C28-C29
2	E	4	LHE	C28-C27-CA-C
2	F	4	LHE	CA-C27-C28-C29
2	E	4	LHE	O-C-CA-N5
2	E	4	LHE	OXT-C-CA-N5
2	E	3	TIH	N-CA-CB-CG
2	F	4	LHE	CA2-C21-C22-C23
2	D	4	LHE	O-C-CA-N5
2	D	4	LHE	CA2-C21-C22-C24
2	D	4	LHE	OXT-C-CA-N5
2	D	3	TIH	CA-CB-CG-CD
2	E	4	LHE	C25-C20-N5-CA
2	D	4	LHE	C-CA-N5-C20
2	E	4	LHE	OXT-C-CA-C27
2	E	3	TIH	C-CA-CB-CG
2	E	4	LHE	O-C-CA-C27
2	D	4	LHE	C25-C20-N5-CA
2	D	4	LHE	C22-C21-CA2-C25
2	F	4	LHE	N5-C20-C25-CA2

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	LHE	1	0
2	E	4	LHE	1	0
2	F	4	LHE	1	0
2	E	3	TIH	1	0
2	D	3	TIH	2	0
2	F	3	TIH	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	389/390 (99%)	-0.16	15 (3%)	39	34	35, 60, 120, 196	0
1	B	389/390 (99%)	-0.04	20 (5%)	28	23	40, 59, 110, 190	0
1	C	390/390 (100%)	0.15	33 (8%)	10	7	35, 64, 138, 192	0
2	D	2/4 (50%)	-0.34	0	100	100	51, 51, 51, 58	0
2	E	2/4 (50%)	-0.57	0	100	100	51, 51, 51, 52	0
2	F	2/4 (50%)	0.11	0	100	100	62, 62, 62, 72	0
All	All	1174/1182 (99%)	-0.02	68 (5%)	23	18	35, 61, 127, 196	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	PHE	15.0
1	C	232	GLY	14.0
1	B	220	PHE	8.7
1	C	222	LEU	7.8
1	C	221	PRO	7.4
1	C	219	GLY	6.8
1	A	221	PRO	6.7
1	C	231	VAL	6.7
1	C	220	PHE	6.7
1	C	224	GLN	6.6
1	A	223	ASN	6.5
1	B	439	ASP	6.5
1	B	440	MET	6.0
1	C	223	ASN	6.0
1	C	229	ALA	5.7
1	C	226	GLU	5.5
1	A	219	GLY	5.5
1	C	225	SER	5.4
1	A	373	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	221	PRO	4.9
1	A	225	SER	4.9
1	B	222	LEU	4.7
1	B	224	GLN	4.6
1	B	223	ASN	4.5
1	B	230	SER	4.3
1	C	230	SER	4.2
1	C	373	VAL	4.1
1	C	227	VAL	4.0
1	C	218	ALA	4.0
1	A	226	GLU	4.0
1	A	374	ALA	3.8
1	A	421	HIS	3.7
1	B	225	SER	3.7
1	B	374	ALA	3.7
1	C	59	SER	3.7
1	C	335	THR	3.7
1	A	222	LEU	3.6
1	A	229	ALA	3.5
1	B	355	GLN	3.4
1	C	378	ASP	3.2
1	C	377	GLN	3.1
1	B	442	ASP	3.0
1	C	58	GLY	3.0
1	B	366	TYR	3.0
1	C	228	LEU	3.0
1	C	330	CYS	2.9
1	C	337	PRO	2.7
1	A	375	THR	2.5
1	C	374	ALA	2.5
1	C	372	ASP	2.5
1	A	420	CYS	2.5
1	B	354	ASN	2.5
1	C	331	TRP	2.5
1	B	438	LEU	2.5
1	B	436	VAL	2.4
1	B	375	THR	2.3
1	C	217	GLY	2.2
1	A	376	SER	2.2
1	B	318	PHE	2.2
1	C	375	THR	2.2
1	B	373	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	369	PRO	2.2
1	B	219	GLY	2.1
1	C	355	GLN	2.1
1	C	315	THR	2.1
1	C	318	PHE	2.0
1	A	230	SER	2.0
1	C	233	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	LHE	E	4	17/17	0.94	0.24	38,52,81,87	0
2	LHE	F	4	17/17	0.94	0.24	42,46,77,81	0
2	TIH	E	3	10/11	0.95	0.16	35,40,44,53	0
2	LHE	D	4	17/17	0.95	0.25	37,45,70,80	0
2	TIH	F	3	10/11	0.96	0.12	47,55,59,69	0
2	TIH	D	3	10/11	0.98	0.13	36,44,47,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.