



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 AM GMT

PDB ID : 3EE6
Title : Crystal Structure Analysis of Tripeptidyl peptidase -I
Authors : Pal, A.; Kraetzner, R.; Grapp, M.; Gruene, T.; Schreiber, K.; Granborg, M.;
Urlaub, H.; Asif, A.R.; Becker, S.; Gartner, J.; Sheldrick, G.M.; Steinfeld, R.
Deposited on : 2008-09-04
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

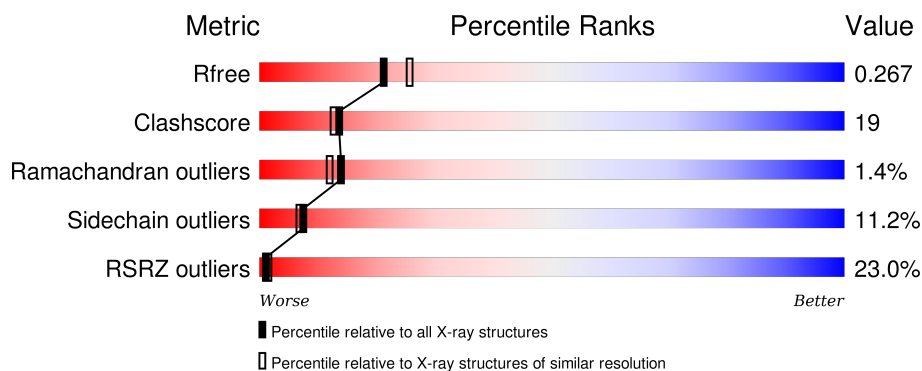
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 $\leq 5\%$. 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	571	
1	B	571	

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
2	NAG	A	575	-	-	-	X
2	NAG	B	575	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8361 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 Tripeptidyl-peptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4082	2588	714	769	11			
1	B	529	Total	C	N	O	S	0	0	0
			4080	2587	714	768	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	564	ARG	-	EXPRESSION TAG	UNP O14773
A	565	SER	-	EXPRESSION TAG	UNP O14773
A	566	HIS	-	EXPRESSION TAG	UNP O14773
A	567	HIS	-	EXPRESSION TAG	UNP O14773
A	568	HIS	-	EXPRESSION TAG	UNP O14773
A	569	HIS	-	EXPRESSION TAG	UNP O14773
A	570	HIS	-	EXPRESSION TAG	UNP O14773
A	571	HIS	-	EXPRESSION TAG	UNP O14773
B	564	ARG	-	EXPRESSION TAG	UNP O14773
B	565	SER	-	EXPRESSION TAG	UNP O14773
B	566	HIS	-	EXPRESSION TAG	UNP O14773
B	567	HIS	-	EXPRESSION TAG	UNP O14773
B	568	HIS	-	EXPRESSION TAG	UNP O14773
B	569	HIS	-	EXPRESSION TAG	UNP O14773
B	570	HIS	-	EXPRESSION TAG	UNP O14773
B	571	HIS	-	EXPRESSION TAG	UNP O14773

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	A	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		
2	B	1	Total	C	N	O	0	0
			13	8	1	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

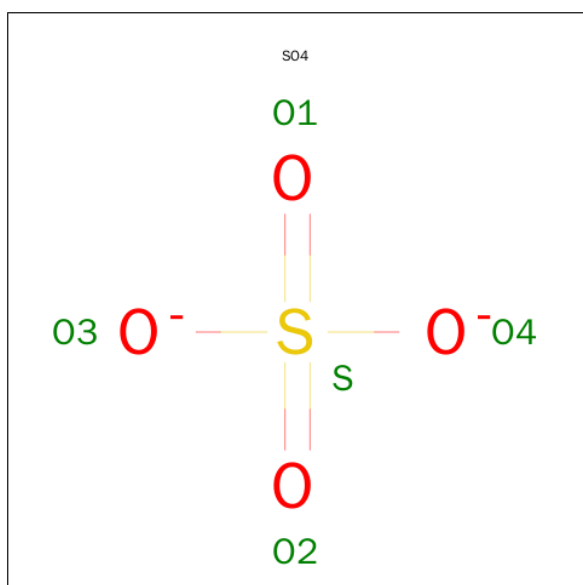
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0

Continued on next page...

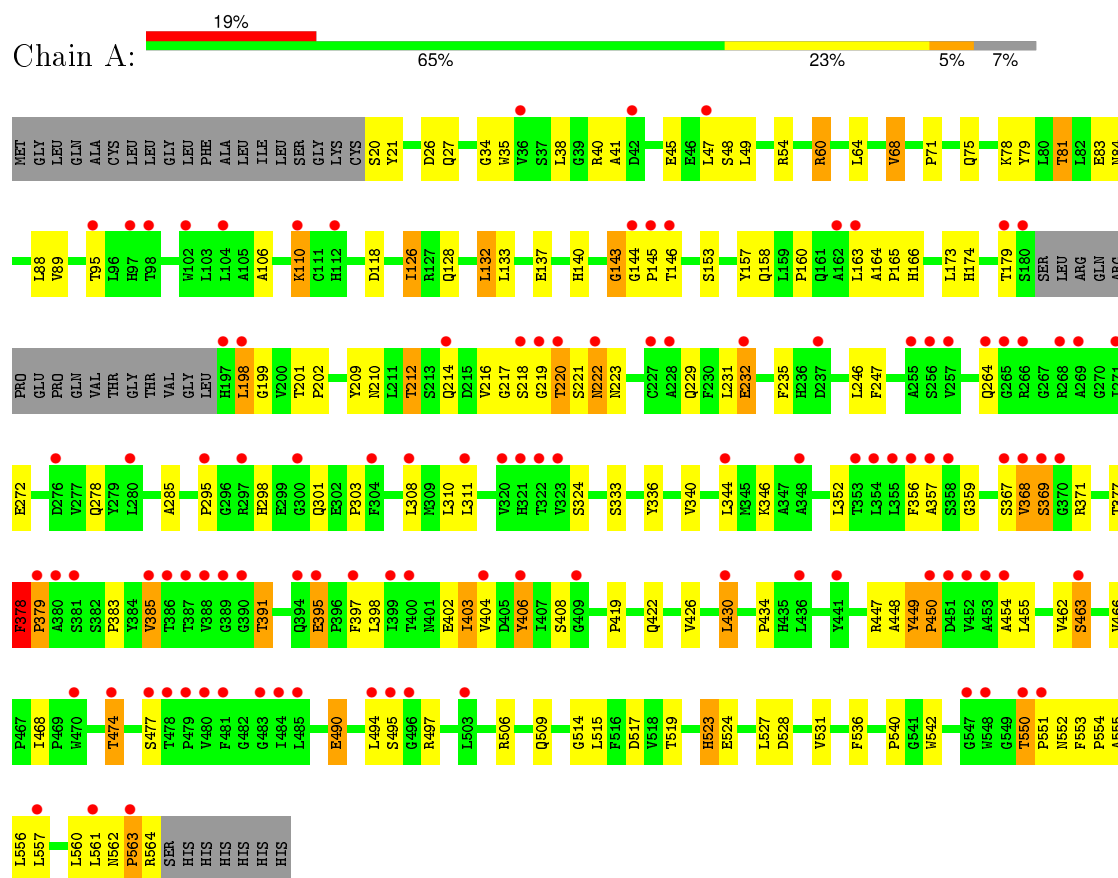
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	37	Total	O	0	0
			37	37		

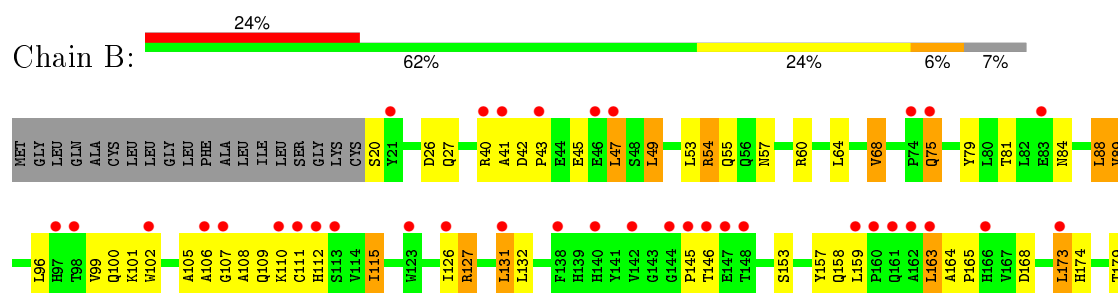
3 Residue-property plots [i](#)

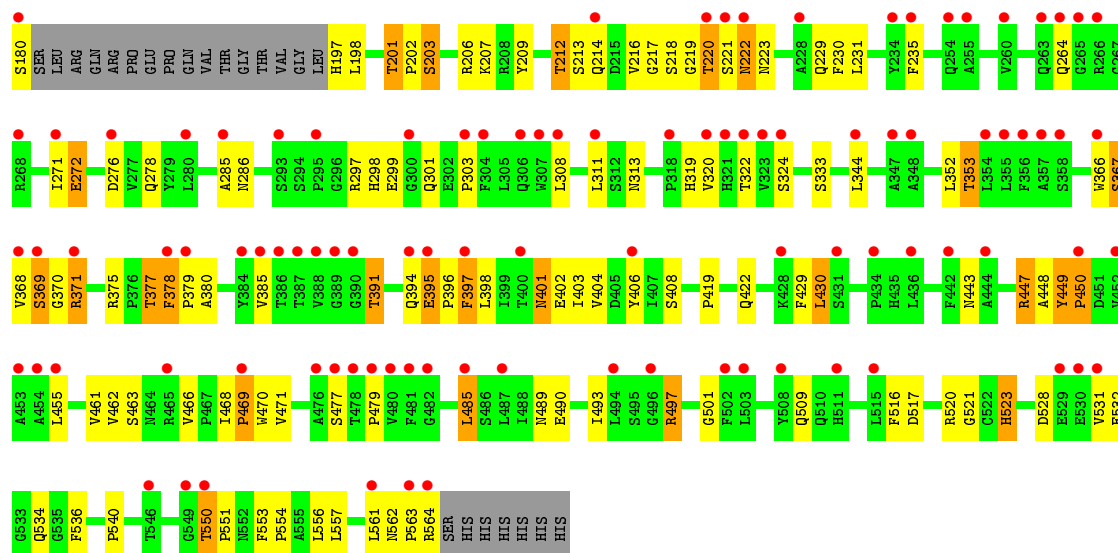
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Tripeptidyl-peptidase 1



• Molecule 1: Tripeptidyl-peptidase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	113.45Å 128.93Å 100.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 2.35 39.21 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.21-2.35) 99.6 (39.21-2.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.218 , 0.262 0.225 , 0.267	Depositor DCC
R_{free} test set	3150 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61780 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8361	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 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, CA, NAG, CL

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	0.52	0/4204	0.75	2/5741 (0.0%)
1	B	0.48	0/4202	0.71	1/5739 (0.0%)
All	All	0.50	0/8406	0.73	3/11480 (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
1	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	PHE	C-N-CD	-9.12	100.54	120.60
1	B	378	PHE	C-N-CD	-7.35	104.42	120.60
1	A	450	PRO	N-CA-C	-5.52	97.75	112.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	PHE	Peptide
1	A	449	TYR	Peptide
1	B	378	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	449	TYR	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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	4082	0	3900	138	0
1	B	4080	0	3901	164	0
2	A	52	0	44	0	0
2	B	52	0	44	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	36	0	0	0	0
7	B	37	0	0	2	0
All	All	8361	0	7889	301	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 19.

All (301) 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:562:ASN:HB3	1:A:563:PRO:CD	1.57	1.33
1:A:562:ASN:CB	1:A:563:PRO:HD3	1.69	1.20
1:A:95:THR:HG22	1:A:166:HIS:ND1	1.56	1.20
1:A:20:SER:OG	1:A:158:GLN:NE2	1.78	1.17
1:B:368:VAL:HG12	1:B:369:SER:H	1.04	1.16
1:A:146:THR:CB	1:A:232:GLU:HG2	1.82	1.09
1:B:563:PRO:O	4:B:580:CL:CL	2.09	1.08
1:B:212:THR:HG22	1:B:214:GLN:H	1.19	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:NH1	1:A:561:LEU:O	1.92	1.03
1:B:101:LYS:HG3	1:B:102:TRP:N	1.71	1.02
1:B:368:VAL:HG12	1:B:369:SER:N	1.71	1.01
1:B:102:TRP:CZ3	1:B:163:LEU:HD11	1.99	0.97
1:B:371:ARG:HH11	1:B:371:ARG:CB	1.77	0.97
1:A:391:THR:HG22	1:A:455:LEU:HA	1.48	0.96
1:B:368:VAL:CG1	1:B:369:SER:H	1.77	0.96
1:A:357:ALA:HB1	1:A:474:THR:HG23	1.48	0.95
1:B:96:LEU:O	1:B:100:GLN:HG3	1.69	0.92
1:A:146:THR:CB	1:A:232:GLU:CG	2.49	0.90
1:B:102:TRP:CE3	1:B:163:LEU:HD11	2.07	0.89
1:A:34:GLY:O	1:A:143:GLY:O	1.90	0.89
1:A:463:SER:O	1:A:466:VAL:HG12	1.72	0.88
1:A:391:THR:HG21	1:A:402:GLU:OE1	1.72	0.87
1:A:562:ASN:HB3	1:A:563:PRO:HD3	0.87	0.87
1:A:368:VAL:HG12	1:A:369:SER:N	1.88	0.86
1:B:422:GLN:HE22	1:B:448:ALA:H	1.23	0.85
1:B:371:ARG:HH11	1:B:371:ARG:HB3	1.41	0.84
1:A:41:ALA:HB1	1:A:126:ILE:HD13	1.60	0.83
1:B:391:THR:HG22	1:B:455:LEU:HA	1.58	0.83
1:A:81:THR:HG22	1:A:84:ASN:H	1.45	0.82
1:B:209:TYR:CE2	1:B:550:THR:HG23	2.15	0.81
1:B:404:VAL:HG22	1:B:521:GLY:HA3	1.60	0.81
1:B:497:ARG:NH1	1:B:561:LEU:HD22	1.96	0.81
1:B:368:VAL:O	1:B:369:SER:C	2.18	0.81
1:B:102:TRP:CE3	1:B:163:LEU:CD1	2.63	0.81
1:B:209:TYR:HE2	1:B:550:THR:CG2	1.93	0.81
1:B:531:VAL:HG12	1:B:531:VAL:O	1.79	0.81
1:B:216:VAL:CG1	1:B:217:GLY:N	2.45	0.80
1:B:209:TYR:CE2	1:B:550:THR:CG2	2.66	0.79
1:A:41:ALA:HB1	1:A:126:ILE:CD1	2.13	0.79
1:B:391:THR:HG21	1:B:402:GLU:OE1	1.81	0.78
1:B:105:ALA:O	1:B:106:ALA:HB3	1.83	0.78
1:B:497:ARG:HH12	1:B:561:LEU:HD22	1.49	0.78
1:B:230:PHE:O	1:B:297:ARG:NH1	2.17	0.77
1:B:81:THR:HG23	1:B:84:ASN:H	1.48	0.77
1:A:357:ALA:HB1	1:A:474:THR:CG2	2.14	0.77
1:A:216:VAL:CG1	1:A:217:GLY:N	2.48	0.77
1:B:127:ARG:O	1:B:131:LEU:HD23	1.86	0.76
1:A:229:GLN:HE22	1:A:231:LEU:HB2	1.48	0.76
1:B:353:THR:HB	1:B:501:GLY:O	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:VAL:HG12	1:A:369:SER:H	1.48	0.76
1:A:41:ALA:CB	1:A:126:ILE:HD13	2.15	0.76
1:B:216:VAL:HG22	1:B:285:ALA:HB3	1.68	0.76
1:A:402:GLU:OE2	1:A:550:THR:HG21	1.85	0.76
1:B:216:VAL:HG12	1:B:217:GLY:N	1.99	0.75
1:B:563:PRO:O	1:B:564:ARG:HB2	1.86	0.75
1:A:517:ASP:OD2	1:A:540:PRO:O	2.04	0.75
1:B:497:ARG:NH2	1:B:561:LEU:O	2.21	0.74
1:B:550:THR:HG23	1:B:551:PRO:HD2	1.69	0.73
1:B:371:ARG:NH1	1:B:371:ARG:CB	2.51	0.73
1:B:497:ARG:HH21	1:B:563:PRO:HA	1.53	0.73
1:B:229:GLN:HE22	1:B:231:LEU:HB2	1.54	0.72
1:A:212:THR:HG23	1:A:214:GLN:H	1.54	0.72
1:B:101:LYS:HG3	1:B:102:TRP:H	1.54	0.72
1:A:422:GLN:HE22	1:A:448:ALA:H	1.34	0.72
1:A:562:ASN:CB	1:A:563:PRO:CD	2.38	0.72
1:B:109:GLN:O	1:B:111:CYS:SG	2.48	0.72
1:B:371:ARG:HH11	1:B:371:ARG:HB2	1.55	0.71
1:B:212:THR:CG2	1:B:214:GLN:H	1.99	0.70
1:B:371:ARG:NH1	1:B:371:ARG:HB2	2.05	0.70
1:A:391:THR:HG22	1:A:455:LEU:CA	2.20	0.70
1:A:157:TYR:CD2	1:A:173:LEU:HD23	2.25	0.70
1:A:527:LEU:HD22	1:B:406:TYR:OH	1.91	0.70
1:A:216:VAL:HG12	1:A:217:GLY:N	2.05	0.70
1:A:81:THR:HG23	1:A:83:GLU:H	1.55	0.70
1:A:198:LEU:HD23	1:A:199:GLY:H	1.57	0.70
1:B:497:ARG:NH1	1:B:561:LEU:CD2	2.56	0.69
1:A:562:ASN:HB3	1:A:563:PRO:HD2	1.72	0.69
1:B:212:THR:HG22	1:B:214:GLN:N	2.01	0.68
1:B:102:TRP:CH2	1:B:163:LEU:HD11	2.29	0.68
1:A:223:ASN:HD22	1:A:490:GLU:HG3	1.59	0.68
1:A:209:TYR:CE2	1:A:550:THR:HG23	2.29	0.68
1:B:402:GLU:OE2	1:B:550:THR:HG21	1.93	0.68
1:A:563:PRO:O	1:A:564:ARG:HG3	1.93	0.68
1:B:201:THR:HG23	1:B:202:PRO:HD2	1.76	0.68
1:B:115:ILE:HD13	1:B:313:ASN:OD1	1.93	0.67
1:A:132:LEU:HD13	1:A:133:LEU:HD21	1.75	0.67
1:B:107:GLY:O	1:B:108:ALA:C	2.32	0.67
1:B:100:GLN:O	1:B:101:LYS:CG	2.43	0.67
1:A:35:TRP:CZ3	1:A:143:GLY:HA2	2.31	0.66
1:A:81:THR:H	1:A:84:ASN:HD22	1.40	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG22	1:B:203:SER:H	1.60	0.66
1:B:517:ASP:OD2	1:B:540:PRO:O	2.14	0.66
1:B:497:ARG:NH2	1:B:563:PRO:HA	2.10	0.66
1:B:209:TYR:HE2	1:B:550:THR:HG21	1.58	0.66
1:A:157:TYR:CD2	1:A:173:LEU:CD2	2.80	0.65
1:B:216:VAL:CG1	1:B:217:GLY:H	2.11	0.64
1:B:217:GLY:O	1:B:286:ASN:HB3	1.96	0.64
1:B:463:SER:O	1:B:466:VAL:HG12	1.97	0.64
1:A:359:GLY:H	1:A:474:THR:HG21	1.62	0.64
1:B:299:GLU:OE1	1:B:299:GLU:N	2.30	0.64
1:A:426:VAL:HG12	1:A:430:LEU:HD22	1.79	0.63
1:A:35:TRP:CE3	1:A:143:GLY:HA2	2.33	0.63
1:B:53:LEU:HD22	1:B:99:VAL:HG21	1.80	0.63
1:B:377:THR:HG22	1:B:380:ALA:HB3	1.81	0.62
1:B:449:TYR:HB2	1:B:450:PRO:HA	1.81	0.62
1:B:531:VAL:HG13	1:B:534:GLN:O	2.00	0.61
1:A:223:ASN:HD22	1:A:490:GLU:CG	2.13	0.61
1:B:497:ARG:HH21	1:B:563:PRO:CA	2.14	0.61
1:B:497:ARG:NH2	1:B:562:ASN:O	2.35	0.60
1:A:132:LEU:HD13	1:A:133:LEU:CD2	2.31	0.60
1:B:531:VAL:CG1	1:B:531:VAL:O	2.47	0.60
1:B:100:GLN:O	1:B:102:TRP:N	2.28	0.59
1:B:367:SER:HA	1:B:371:ARG:O	2.03	0.59
1:B:368:VAL:CG1	1:B:369:SER:N	2.43	0.59
1:A:563:PRO:O	4:A:580:CL:CL	2.57	0.59
1:B:57:ASN:HB2	1:B:88:LEU:HD22	1.84	0.58
1:A:132:LEU:C	1:A:133:LEU:HD23	2.24	0.58
1:A:563:PRO:O	1:A:564:ARG:CG	2.51	0.58
1:B:223:ASN:HD22	1:B:490:GLU:HG3	1.69	0.58
1:A:144:GLY:O	1:A:146:THR:N	2.37	0.58
1:B:216:VAL:HG13	1:B:217:GLY:H	1.67	0.58
1:A:216:VAL:CG1	1:A:217:GLY:H	2.15	0.57
1:A:298:HIS:CD2	1:A:298:HIS:H	2.21	0.57
1:B:197:HIS:HA	1:B:396:PRO:O	2.04	0.57
1:A:422:GLN:NE2	1:A:448:ALA:H	2.00	0.57
1:B:229:GLN:HE21	1:B:272:GLU:HG2	1.69	0.57
1:B:466:VAL:HG13	1:B:468:ILE:HD11	1.87	0.57
1:A:466:VAL:HG13	1:A:468:ILE:HD11	1.87	0.56
1:A:368:VAL:CG1	1:A:369:SER:H	2.12	0.56
1:A:216:VAL:HG13	1:A:217:GLY:H	1.70	0.56
1:B:489:ASN:O	1:B:493:ILE:HG23	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:O	1:B:220:THR:N	2.39	0.56
1:A:308:LEU:HD21	1:A:340:VAL:HG13	1.86	0.56
1:B:101:LYS:CG	1:B:102:TRP:N	2.56	0.56
1:B:102:TRP:CD2	1:B:163:LEU:HD11	2.40	0.56
1:B:391:THR:HG22	1:B:455:LEU:CA	2.33	0.56
1:A:144:GLY:C	1:A:146:THR:N	2.57	0.56
1:B:320:VAL:HG22	1:B:353:THR:HG23	1.88	0.55
1:A:45:GLU:HB3	1:A:126:ILE:HD12	1.88	0.55
1:A:110:LYS:CE	1:A:110:LYS:HA	2.37	0.55
1:B:201:THR:HG22	1:B:203:SER:N	2.22	0.54
1:B:20:SER:OG	1:B:158:GLN:NE2	2.41	0.54
1:B:212:THR:CG2	1:B:213:SER:N	2.70	0.54
1:A:216:VAL:HG22	1:A:285:ALA:HB3	1.90	0.54
1:A:95:THR:CG2	1:A:166:HIS:ND1	2.50	0.54
1:B:229:GLN:NE2	1:B:272:GLU:HG2	2.22	0.54
1:A:110:LYS:HE3	1:A:110:LYS:HA	1.89	0.54
1:B:102:TRP:CD2	1:B:163:LEU:CD1	2.90	0.53
1:B:404:VAL:CG2	1:B:521:GLY:HA3	2.37	0.53
1:B:550:THR:HG23	1:B:551:PRO:CD	2.38	0.53
1:A:550:THR:HG23	1:A:551:PRO:HD2	1.90	0.53
1:B:41:ALA:HB3	1:B:126:ILE:HD13	1.90	0.53
1:A:145:PRO:HD2	1:A:179:THR:HG23	1.91	0.52
1:B:216:VAL:HG13	1:B:286:ASN:H	1.75	0.52
1:B:216:VAL:HG22	1:B:285:ALA:CB	2.36	0.52
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.74	0.52
1:B:100:GLN:O	1:B:101:LYS:HG2	2.09	0.52
1:A:81:THR:HG23	1:A:83:GLU:N	2.24	0.52
1:A:160:PRO:HG2	1:A:163:LEU:HD23	1.92	0.52
1:A:201:THR:CG2	1:A:202:PRO:HD2	2.40	0.52
1:A:40:ARG:CZ	1:A:137:GLU:HG3	2.40	0.52
1:A:367:SER:HA	1:A:371:ARG:O	2.09	0.51
1:B:153:SER:O	1:B:174:HIS:HD2	1.92	0.51
1:A:20:SER:OG	1:A:158:GLN:CD	2.46	0.51
1:A:209:TYR:CE2	1:A:550:THR:CG2	2.93	0.51
1:A:146:THR:CB	1:A:232:GLU:OE2	2.59	0.51
1:A:383:PRO:HB3	1:A:419:PRO:HG3	1.93	0.51
1:A:81:THR:HG22	1:A:84:ASN:N	2.21	0.51
1:A:556:LEU:HD22	1:A:560:LEU:HD12	1.92	0.50
1:A:494:LEU:O	1:A:495:SER:CB	2.60	0.50
1:A:218:SER:O	1:A:220:THR:N	2.44	0.49
1:B:102:TRP:CZ3	1:B:163:LEU:CD1	2.82	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:H	1:A:84:ASN:ND2	2.08	0.49
1:A:336:TYR:O	1:A:340:VAL:HG23	2.12	0.49
1:A:359:GLY:N	1:A:474:THR:HG21	2.26	0.49
1:A:71:PRO:HG2	1:A:509:GLN:NE2	2.28	0.49
1:B:397:PHE:C	1:B:398:LEU:HD22	2.33	0.49
1:B:27:GLN:HB2	1:B:333:SER:HB3	1.95	0.49
1:A:295:PRO:O	1:A:303:PRO:HA	2.13	0.49
1:A:402:GLU:O	1:A:403:ILE:HD12	2.12	0.49
1:B:153:SER:O	1:B:174:HIS:CD2	2.66	0.49
1:B:298:HIS:HB3	1:B:299:GLU:OE1	2.13	0.48
1:A:201:THR:HG23	1:A:202:PRO:HD2	1.95	0.48
1:A:278:GLN:HE22	1:A:462:VAL:H	1.59	0.48
1:A:209:TYR:HE2	1:A:550:THR:CG2	2.27	0.48
1:A:27:GLN:HB2	1:A:333:SER:HB3	1.96	0.48
1:A:514:GLY:HA2	1:A:555:ALA:HB1	1.96	0.48
1:A:146:THR:CB	1:A:232:GLU:CB	2.91	0.48
1:A:201:THR:HG22	1:A:202:PRO:N	2.29	0.48
1:B:408:SER:O	1:B:523:HIS:HD2	1.97	0.48
1:A:391:THR:HG23	1:A:455:LEU:HD23	1.96	0.48
1:B:81:THR:HG22	1:B:84:ASN:ND2	2.29	0.48
1:B:319:HIS:CD2	7:B:617:HOH:O	2.66	0.48
1:A:391:THR:CG2	1:A:455:LEU:HD23	2.44	0.47
1:B:398:LEU:N	1:B:398:LEU:HD22	2.28	0.47
1:B:516:PHE:N	1:B:550:THR:O	2.46	0.47
1:B:100:GLN:C	1:B:102:TRP:H	2.17	0.47
1:A:81:THR:CG2	1:A:84:ASN:H	2.23	0.47
1:A:528:ASP:C	1:A:528:ASP:OD1	2.52	0.47
1:B:54:ARG:NH1	1:B:168:ASP:OD1	2.48	0.47
1:B:497:ARG:NH2	1:B:563:PRO:CA	2.76	0.47
1:B:447:ARG:NH1	1:B:448:ALA:O	2.44	0.47
1:A:356:PHE:CE2	1:A:385:VAL:HG21	2.50	0.47
1:B:47:LEU:HD22	1:B:49:LEU:HD13	1.96	0.47
1:B:100:GLN:C	1:B:102:TRP:N	2.67	0.47
1:B:212:THR:HG23	1:B:213:SER:N	2.30	0.47
1:A:519:THR:CG2	1:A:519:THR:O	2.63	0.47
1:B:366:TRP:HB2	1:B:375:ARG:HB2	1.97	0.47
1:A:41:ALA:CB	1:A:126:ILE:CD1	2.86	0.47
1:B:101:LYS:CG	1:B:102:TRP:H	2.27	0.46
1:A:221:SER:OG	1:A:222:ASN:N	2.48	0.46
1:A:378:PHE:CD1	1:A:379:PRO:HA	2.51	0.46
1:B:216:VAL:CG1	1:B:286:ASN:HB2	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:C	1:B:299:GLU:H	2.17	0.46
1:A:201:THR:HG23	1:A:247:PHE:CD1	2.50	0.46
1:A:157:TYR:CE2	1:A:173:LEU:HD22	2.50	0.46
1:B:561:LEU:C	1:B:562:ASN:O	2.51	0.46
1:B:553:PHE:HB3	1:B:554:PRO:HD3	1.97	0.46
1:B:206:ARG:NH2	1:B:285:ALA:HB2	2.30	0.46
1:B:297:ARG:C	1:B:299:GLU:N	2.68	0.46
1:A:519:THR:HG22	1:A:519:THR:O	2.14	0.46
1:A:406:TYR:CZ	1:A:524:GLU:HB3	2.51	0.46
1:B:109:GLN:O	1:B:110:LYS:C	2.55	0.45
1:B:201:THR:HG23	1:B:202:PRO:CD	2.44	0.45
1:B:485:LEU:HA	1:B:485:LEU:HD12	1.85	0.45
1:A:368:VAL:CG1	1:A:369:SER:N	2.57	0.45
1:B:105:ALA:O	1:B:106:ALA:CB	2.50	0.45
1:B:301:GLN:O	1:B:303:PRO:HD3	2.16	0.45
1:B:271:ILE:HD12	1:B:471:VAL:CG2	2.47	0.45
1:A:398:LEU:N	1:A:398:LEU:HD22	2.31	0.45
1:B:562:ASN:O	1:B:563:PRO:C	2.54	0.45
1:A:68:VAL:HG13	1:A:79:TYR:CE1	2.52	0.45
1:B:102:TRP:CE2	1:B:132:LEU:HD21	2.52	0.45
1:A:357:ALA:CB	1:A:474:THR:HG23	2.33	0.45
1:B:377:THR:HB	7:B:629:HOH:O	2.15	0.45
1:A:145:PRO:CD	1:A:179:THR:HG23	2.47	0.45
1:A:556:LEU:HD22	1:A:560:LEU:CD1	2.47	0.45
1:A:553:PHE:HB3	1:A:554:PRO:HD3	1.99	0.45
1:B:41:ALA:CB	1:B:126:ILE:HD13	2.47	0.44
1:A:408:SER:O	1:A:523:HIS:HD2	2.00	0.44
1:A:153:SER:O	1:A:174:HIS:HD2	2.00	0.44
1:A:514:GLY:HA2	1:A:555:ALA:CB	2.47	0.44
1:A:41:ALA:HB3	1:A:126:ILE:HD13	1.96	0.44
1:A:523:HIS:HE1	1:A:536:PHE:H	1.64	0.44
1:B:419:PRO:HD2	1:B:422:GLN:NE2	2.33	0.44
1:B:395:GLU:CD	1:B:398:LEU:HB2	2.38	0.44
1:A:449:TYR:CD1	1:A:449:TYR:C	2.90	0.44
1:A:454:ALA:HB3	1:A:477:SER:HB2	1.99	0.44
1:B:369:SER:HB2	1:B:370:GLY:H	1.66	0.44
1:A:118:ASP:OD2	1:A:346:LYS:NZ	2.50	0.44
1:A:60:ARG:HD3	1:A:60:ARG:HA	1.74	0.44
1:B:278:GLN:HE22	1:B:462:VAL:H	1.65	0.44
1:B:157:TYR:CD2	1:B:173:LEU:HD22	2.53	0.43
1:B:528:ASP:O	1:B:532:GLU:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ALA:N	1:B:165:PRO:CD	2.81	0.43
1:B:563:PRO:O	1:B:564:ARG:CB	2.56	0.43
1:B:404:VAL:HG21	1:B:521:GLY:C	2.38	0.43
1:B:75:GLN:CA	1:B:75:GLN:HE21	2.31	0.43
1:B:20:SER:HB2	1:B:159:LEU:O	2.18	0.43
1:A:26:ASP:N	1:A:26:ASP:OD2	2.50	0.43
1:B:394:GLN:HE21	1:B:401:ASN:HB3	1.84	0.43
1:A:216:VAL:HG13	1:A:285:ALA:O	2.17	0.43
1:A:210:ASN:ND2	1:A:552:ASN:OD1	2.51	0.43
1:B:229:GLN:HG3	1:B:272:GLU:HG3	2.00	0.43
1:A:132:LEU:CD1	1:A:133:LEU:HD21	2.46	0.43
1:B:469:PRO:HB2	1:B:470:TRP:CD1	2.54	0.43
1:A:128:GLN:O	1:A:132:LEU:HB2	2.19	0.43
1:B:497:ARG:NH2	1:B:562:ASN:C	2.72	0.43
1:B:81:THR:HG22	1:B:84:ASN:CG	2.38	0.43
1:B:26:ASP:OD2	1:B:26:ASP:N	2.52	0.43
1:A:448:ALA:HB1	1:A:542:TRP:HH2	1.83	0.42
1:A:301:GLN:O	1:A:303:PRO:HD3	2.19	0.42
1:A:395:GLU:CD	1:A:398:LEU:HB2	2.40	0.42
1:B:68:VAL:HG13	1:B:79:TYR:CE1	2.55	0.42
1:B:429:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
1:A:21:TYR:O	1:A:158:GLN:CB	2.68	0.42
1:B:523:HIS:HE1	1:B:536:PHE:H	1.68	0.42
1:B:221:SER:OG	1:B:222:ASN:N	2.52	0.42
1:B:561:LEU:O	1:B:562:ASN:C	2.55	0.41
1:A:391:THR:HG22	1:A:455:LEU:N	2.34	0.41
1:B:42:ASP:O	1:B:43:PRO:C	2.58	0.41
1:A:298:HIS:N	1:A:298:HIS:CD2	2.85	0.41
1:B:198:LEU:HD11	1:B:397:PHE:O	2.21	0.41
1:A:515:LEU:HD23	1:A:551:PRO:HA	2.01	0.41
1:B:320:VAL:HG22	1:B:353:THR:CG2	2.50	0.41
1:B:45:GLU:O	1:B:126:ILE:HG23	2.19	0.41
1:B:403:ILE:HG13	1:B:520:ARG:HB3	2.03	0.41
1:A:21:TYR:O	1:A:158:GLN:HB2	2.20	0.41
1:A:164:ALA:N	1:A:165:PRO:CD	2.84	0.41
1:B:297:ARG:O	1:B:299:GLU:N	2.54	0.41
1:A:144:GLY:O	1:A:146:THR:C	2.59	0.41
1:A:41:ALA:HA	1:A:140:HIS:CE1	2.56	0.41
1:B:201:THR:CG2	1:B:202:PRO:N	2.84	0.41
1:A:106:ALA:HB2	1:A:132:LEU:HD23	2.01	0.41
1:B:408:SER:O	1:B:523:HIS:CD2	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:HB3	1:B:89:VAL:HG22	2.02	0.41
1:B:229:GLN:HE21	1:B:231:LEU:HG	1.86	0.41
1:A:463:SER:O	1:A:466:VAL:CG1	2.56	0.40
1:B:322:THR:HG21	1:B:479:PRO:HA	2.02	0.40
1:B:179:THR:O	1:B:180:SER:C	2.60	0.40
1:B:556:LEU:HA	1:B:556:LEU:HD23	1.94	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	525/571 (92%)	495 (94%)	21 (4%)	9 (2%)	11	9
1	B	525/571 (92%)	479 (91%)	40 (8%)	6 (1%)	17	17
All	All	1050/1142 (92%)	974 (93%)	61 (6%)	15 (1%)	14	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLY
1	A	368	VAL
1	B	219	GLY
1	B	369	SER
1	A	406	TYR
1	A	450	PRO
1	A	563	PRO
1	B	379	PRO
1	A	369	SER
1	B	450	PRO
1	A	379	PRO
1	A	434	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	145	PRO
1	A	143	GLY
1	B	469	PRO

5.3.2 Protein sidechains ⓘ

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	443/479 (92%)	396 (89%)	47 (11%)	8	8
1	B	443/479 (92%)	391 (88%)	52 (12%)	7	6
All	All	886/958 (92%)	787 (89%)	99 (11%)	7	7

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	47	LEU
1	A	48	SER
1	A	49	LEU
1	A	54	ARG
1	A	60	ARG
1	A	64	LEU
1	A	68	VAL
1	A	75	GLN
1	A	78	LYS
1	A	81	THR
1	A	88	LEU
1	A	89	VAL
1	A	110	LYS
1	A	126	ILE
1	A	132	LEU
1	A	198	LEU
1	A	212	THR
1	A	220	THR
1	A	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	GLU
1	A	235	PHE
1	A	246	LEU
1	A	264	GLN
1	A	272	GLU
1	A	310	LEU
1	A	311	LEU
1	A	324	SER
1	A	344	LEU
1	A	352	LEU
1	A	377	THR
1	A	385	VAL
1	A	391	THR
1	A	395	GLU
1	A	397	PHE
1	A	403	ILE
1	A	404	VAL
1	A	430	LEU
1	A	447	ARG
1	A	463	SER
1	A	474	THR
1	A	490	GLU
1	A	506	ARG
1	A	523	HIS
1	A	531	VAL
1	A	550	THR
1	A	557	LEU
1	B	40	ARG
1	B	47	LEU
1	B	49	LEU
1	B	54	ARG
1	B	60	ARG
1	B	64	LEU
1	B	68	VAL
1	B	75	GLN
1	B	88	LEU
1	B	89	VAL
1	B	112	HIS
1	B	115	ILE
1	B	127	ARG
1	B	131	LEU
1	B	146	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	LEU
1	B	173	LEU
1	B	201	THR
1	B	203	SER
1	B	207	LYS
1	B	212	THR
1	B	220	THR
1	B	222	ASN
1	B	235	PHE
1	B	264	GLN
1	B	272	GLU
1	B	276	ASP
1	B	308	LEU
1	B	311	LEU
1	B	324	SER
1	B	344	LEU
1	B	352	LEU
1	B	353	THR
1	B	367	SER
1	B	371	ARG
1	B	377	THR
1	B	385	VAL
1	B	391	THR
1	B	395	GLU
1	B	397	PHE
1	B	401	ASN
1	B	430	LEU
1	B	443	ASN
1	B	447	ARG
1	B	461	VAL
1	B	477	SER
1	B	485	LEU
1	B	497	ARG
1	B	509	GLN
1	B	523	HIS
1	B	550	THR
1	B	557	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	GLN
1	A	84	ASN
1	A	158	GLN
1	A	161	GLN
1	A	174	HIS
1	A	223	ASN
1	A	225	GLN
1	A	229	GLN
1	A	278	GLN
1	A	298	HIS
1	A	321	HIS
1	A	394	GLN
1	A	422	GLN
1	A	504	ASN
1	A	509	GLN
1	A	523	HIS
1	B	56	GLN
1	B	57	ASN
1	B	75	GLN
1	B	100	GLN
1	B	158	GLN
1	B	174	HIS
1	B	223	ASN
1	B	225	GLN
1	B	229	GLN
1	B	254	GLN
1	B	264	GLN
1	B	278	GLN
1	B	394	GLN
1	B	422	GLN
1	B	504	ASN
1	B	509	GLN
1	B	523	HIS
1	B	552	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 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	NAG	A	572	1	13,13,15	0.98	0	13,17,21	1.19	2 (15%)
2	NAG	A	573	1	13,13,15	1.54	2 (15%)	13,17,21	2.62	5 (38%)
2	NAG	A	574	1	13,13,15	0.87	0	13,17,21	1.16	2 (15%)
2	NAG	A	575	1	13,13,15	0.75	0	13,17,21	1.22	1 (7%)
6	SO4	A	582	-	4,4,4	0.17	0	6,6,6	0.26	0
2	NAG	B	572	1	13,13,15	0.94	0	13,17,21	1.62	4 (30%)
2	NAG	B	573	1	13,13,15	0.97	0	13,17,21	1.34	3 (23%)
2	NAG	B	574	1	13,13,15	1.22	1 (7%)	13,17,21	1.74	3 (23%)
2	NAG	B	575	1	13,13,15	0.95	0	13,17,21	1.22	2 (15%)
6	SO4	B	582	-	4,4,4	0.18	0	6,6,6	0.20	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	NAG	A	572	1	-	0/6/19/26	1/1/1/1
2	NAG	A	573	1	-	0/6/19/26	0/1/1/1
2	NAG	A	574	1	-	0/6/19/26	0/1/1/1
2	NAG	A	575	1	-	0/6/19/26	0/1/1/1
6	SO4	A	582	-	-	0/0/0/0	0/0/0/0
2	NAG	B	572	1	-	0/6/19/26	1/1/1/1
2	NAG	B	573	1	-	0/6/19/26	0/1/1/1
2	NAG	B	574	1	-	0/6/19/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	575	1	-	0/6/19/26	0/1/1/1
6	SO4	B	582	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	574	NAG	C4-C3	2.81	1.57	1.52
2	A	573	NAG	C4-C3	3.04	1.57	1.52
2	A	573	NAG	C3-C2	3.73	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	573	NAG	C3-C4-C5	-4.02	103.25	111.40
2	B	572	NAG	O3-C3-C2	-2.69	105.13	110.48
2	B	572	NAG	C3-C4-C5	-2.47	106.38	111.40
2	A	573	NAG	O7-C7-C8	-2.42	117.62	122.06
2	B	574	NAG	O3-C3-C2	-2.18	106.16	110.48
2	B	573	NAG	O3-C3-C2	-2.06	106.39	110.48
2	A	574	NAG	C4-C3-C2	2.03	114.15	111.34
2	B	573	NAG	C4-C5-C6	2.09	116.22	112.38
2	B	574	NAG	O5-C5-C6	2.15	109.20	106.51
2	B	572	NAG	C4-C3-C2	2.16	114.33	111.34
2	B	573	NAG	O5-C5-C4	2.23	113.30	108.86
2	B	575	NAG	O5-C5-C4	2.25	113.34	108.86
2	A	572	NAG	C4-C5-C6	2.26	116.53	112.38
2	B	572	NAG	O5-C5-C6	2.29	109.37	106.51
2	A	574	NAG	O5-C5-C4	2.36	113.57	108.86
2	A	572	NAG	O5-C5-C6	2.46	109.58	106.51
2	B	575	NAG	C4-C3-C2	2.67	115.03	111.34
2	A	573	NAG	O5-C5-C4	3.14	115.12	108.86
2	A	575	NAG	O5-C5-C6	3.15	110.45	106.51
2	A	573	NAG	C2-N2-C7	3.69	127.79	123.04
2	B	574	NAG	C4-C3-C2	4.39	117.41	111.34
2	A	573	NAG	C4-C3-C2	5.12	118.42	111.34

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	572	NAG	C1-C2-C3-C4-C5-O5
2	A	572	NAG	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	529/571 (92%)	1.20	108 (20%)	1 2	49, 67, 79, 88	0
1	B	529/571 (92%)	1.32	135 (25%)	1 1	60, 67, 79, 91	0
All	All	1058/1142 (92%)	1.26	243 (22%)	1 1	49, 67, 79, 91	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	THR	14.9
1	A	220	THR	11.6
1	A	388	VAL	8.3
1	A	255	ALA	8.1
1	A	265	GLY	8.0
1	A	198	LEU	7.6
1	B	369	SER	7.1
1	B	531	VAL	7.1
1	B	397	PHE	6.9
1	A	496	GLY	6.8
1	B	355	LEU	6.7
1	A	145	PRO	6.6
1	B	145	PRO	6.5
1	A	264	GLN	6.4
1	A	355	LEU	6.3
1	B	123	TRP	6.1
1	B	368	VAL	5.8
1	B	480	VAL	5.7
1	B	563	PRO	5.6
1	A	399	ILE	5.5
1	A	368	VAL	5.4
1	A	452	VAL	5.4
1	B	564	ARG	5.4
1	A	354	LEU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	5.3
1	B	395	GLU	5.2
1	B	400	THR	5.1
1	B	323	VAL	5.0
1	B	180	SER	4.9
1	B	356	PHE	4.8
1	B	453	ALA	4.8
1	B	308	LEU	4.8
1	A	387	THR	4.8
1	B	477	SER	4.6
1	A	222	ASN	4.6
1	A	369	SER	4.6
1	A	563	PRO	4.6
1	B	214	GLN	4.5
1	A	454	ALA	4.4
1	A	478	THR	4.4
1	A	323	VAL	4.3
1	B	388	VAL	4.3
1	A	551	PRO	4.2
1	A	280	LEU	4.2
1	A	477	SER	4.2
1	A	162	ALA	4.2
1	A	453	ALA	4.1
1	A	295	PRO	4.1
1	A	480	VAL	4.1
1	B	163	LEU	4.0
1	B	386	THR	4.0
1	A	197	HIS	4.0
1	B	371	ARG	4.0
1	A	344	LEU	4.0
1	B	479	PRO	4.0
1	B	160	PRO	4.0
1	A	481	PHE	4.0
1	A	397	PHE	3.9
1	A	300	GLY	3.9
1	A	180	SER	3.9
1	B	454	ALA	3.9
1	A	400	THR	3.8
1	B	387	THR	3.8
1	B	102	TRP	3.8
1	B	322	THR	3.8
1	B	146	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	265	GLY	3.7
1	B	21	TYR	3.7
1	A	451	ASP	3.7
1	A	389	GLY	3.7
1	B	254	GLN	3.7
1	A	219	GLY	3.7
1	A	385	VAL	3.7
1	B	112	HIS	3.7
1	B	260	VAL	3.7
1	A	386	THR	3.6
1	B	234	TYR	3.6
1	A	112	HIS	3.6
1	A	450	PRO	3.6
1	A	485	LEU	3.6
1	B	264	GLN	3.6
1	B	494	LEU	3.6
1	B	496	GLY	3.5
1	B	354	LEU	3.5
1	B	481	PHE	3.5
1	A	547	GLY	3.5
1	A	110	LYS	3.5
1	B	97	HIS	3.5
1	A	256	SER	3.4
1	A	494	LEU	3.4
1	B	147	GLU	3.4
1	B	222	ASN	3.4
1	A	214	GLN	3.4
1	B	142	VAL	3.3
1	B	311	LEU	3.3
1	A	356	PHE	3.3
1	A	104	LEU	3.3
1	A	479	PRO	3.3
1	A	394	GLN	3.3
1	B	221	SER	3.3
1	B	110	LYS	3.2
1	B	357	ALA	3.2
1	A	232	GLU	3.2
1	B	348	ALA	3.2
1	A	268	ARG	3.2
1	A	321	HIS	3.1
1	B	295	PRO	3.1
1	A	218	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	GLY	3.1
1	B	148	THR	3.1
1	B	389	GLY	3.1
1	B	307	TRP	3.1
1	B	530	GLU	3.0
1	B	366	TRP	3.0
1	A	146	THR	3.0
1	A	320	VAL	3.0
1	A	483	GLY	3.0
1	B	561	LEU	3.0
1	B	478	THR	3.0
1	A	406	TYR	3.0
1	B	46	GLU	3.0
1	A	269	ALA	3.0
1	A	484	ILE	3.0
1	B	107	GLY	2.9
1	B	406	TYR	2.9
1	B	321	HIS	2.9
1	B	138	PHE	2.9
1	A	503	LEU	2.9
1	B	436	LEU	2.9
1	A	390	GLY	2.9
1	A	97	HIS	2.9
1	B	379	PRO	2.9
1	B	159	LEU	2.9
1	B	75	GLN	2.9
1	B	347	ALA	2.8
1	B	74	PRO	2.8
1	B	131	LEU	2.8
1	B	358	SER	2.8
1	A	102	TRP	2.8
1	B	550	THR	2.8
1	B	455	LEU	2.8
1	B	228	ALA	2.8
1	A	95	THR	2.8
1	A	308	LEU	2.8
1	A	561	LEU	2.7
1	B	285	ALA	2.7
1	B	378	PHE	2.7
1	B	304	PHE	2.7
1	B	166	HIS	2.7
1	B	390	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	348	ALA	2.6
1	B	442	PHE	2.6
1	A	266	ARG	2.6
1	A	370	GLY	2.6
1	B	385	VAL	2.6
1	B	271	ILE	2.6
1	B	255	ALA	2.6
1	A	322	THR	2.6
1	B	111	CYS	2.6
1	B	144	GLY	2.6
1	B	549	GLY	2.6
1	A	550	THR	2.6
1	B	113	SER	2.5
1	B	320	VAL	2.5
1	B	546	THR	2.5
1	B	324	SER	2.5
1	B	469	PRO	2.5
1	B	452	VAL	2.5
1	B	476	ALA	2.5
1	B	503	LEU	2.5
1	B	266	ARG	2.5
1	B	98	THR	2.5
1	A	304	PHE	2.5
1	B	106	ALA	2.4
1	B	431	SER	2.4
1	A	47	LEU	2.4
1	A	276	ASP	2.4
1	B	434	PRO	2.4
1	B	502	PHE	2.4
1	B	344	LEU	2.4
1	B	263	GLN	2.4
1	A	237	ASP	2.4
1	B	161	GLN	2.4
1	A	42	ASP	2.4
1	B	276	ASP	2.4
1	B	465	ARG	2.4
1	B	384	TYR	2.4
1	A	357	ALA	2.4
1	B	444	ALA	2.3
1	B	482	GLY	2.3
1	A	358	SER	2.3
1	B	306	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	529	GLU	2.3
1	A	463	SER	2.3
1	A	557	LEU	2.3
1	A	395	GLU	2.3
1	A	380	ALA	2.3
1	B	140	HIS	2.3
1	B	428	LYS	2.3
1	A	311	LEU	2.3
1	B	515	LEU	2.3
1	A	227	CYS	2.2
1	B	162	ALA	2.2
1	B	47	LEU	2.2
1	B	394	GLN	2.2
1	A	379	PRO	2.2
1	B	43	PRO	2.2
1	B	40	ARG	2.2
1	A	144	GLY	2.2
1	A	495	SER	2.2
1	A	36	VAL	2.2
1	B	235	PHE	2.2
1	A	271	ILE	2.2
1	A	441	TYR	2.2
1	B	83	GLU	2.2
1	B	280	LEU	2.2
1	A	228	ALA	2.2
1	A	548	TRP	2.1
1	B	485	LEU	2.1
1	A	257	VAL	2.1
1	A	404	VAL	2.1
1	B	318	PRO	2.1
1	A	98	THR	2.1
1	A	179	THR	2.1
1	A	409	GLY	2.1
1	B	41	ALA	2.1
1	B	450	PRO	2.1
1	A	353	THR	2.1
1	A	436	LEU	2.1
1	B	487	LEU	2.1
1	A	297	ARG	2.1
1	B	126	ILE	2.1
1	A	470	TRP	2.0
1	A	367	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	381	SER	2.0
1	B	293	SER	2.0
1	B	303	PRO	2.0
1	A	474	THR	2.0
1	A	430	LEU	2.0
1	B	173	LEU	2.0
1	B	508	TYR	2.0
1	B	511	HIS	2.0
1	B	268	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	NAG	A	575	13/15	0.22	0.42	4.77	87,88,90,91	0
2	NAG	B	575	13/15	0.53	0.44	4.42	88,90,93,93	0
4	CL	A	580	1/1	0.88	0.27	0.53	98,98,98,98	0
2	NAG	A	573	13/15	0.74	0.21	0.09	68,72,79,80	0
2	NAG	A	572	13/15	0.77	0.20	-0.34	82,85,89,90	0
2	NAG	A	574	13/15	0.85	0.16	-0.41	80,81,84,85	0
2	NAG	B	573	13/15	0.85	0.19	-0.50	69,74,79,80	0
4	CL	B	580	1/1	0.88	0.20	-0.63	112,112,112,112	0
2	NAG	B	572	13/15	0.90	0.09	-1.79	72,73,77,78	0
5	CA	A	581	1/1	0.98	0.04	-2.16	66,66,66,66	0
5	CA	B	581	1/1	0.92	0.07	-2.65	61,61,61,61	0
6	SO4	B	582	5/5	0.84	0.30	-	104,104,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	B	577	1/1	0.96	0.09	-	94,94,94,94	0
3	ZN	A	577	1/1	0.95	0.06	-	71,71,71,71	1
3	ZN	A	576	1/1	0.94	0.14	-	91,91,91,91	0
6	SO4	A	582	5/5	0.84	0.40	-	112,112,112,112	0
3	ZN	B	579	1/1	0.74	0.29	-	116,116,116,116	0
2	NAG	B	574	13/15	0.78	0.22	-	81,83,85,85	0
3	ZN	B	578	1/1	0.97	0.09	-	90,90,90,90	0
3	ZN	A	578	1/1	0.97	0.18	-	83,83,83,83	0
3	ZN	B	576	1/1	0.80	0.09	-	87,87,87,87	1
3	ZN	A	579	1/1	0.81	0.11	-	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.