Full wwPDB X-ray Structure Validation Report

Oct 25, 2016 – 03:21 PM EDT

PDB ID	:	5L1H
Title	:	AMPA subtype ionotropic glutamate receptor GluA2 in complex with non-competitive inhibitor GYKI53655
Authors	:	Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.
Deposited on	:	2016-07-29
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

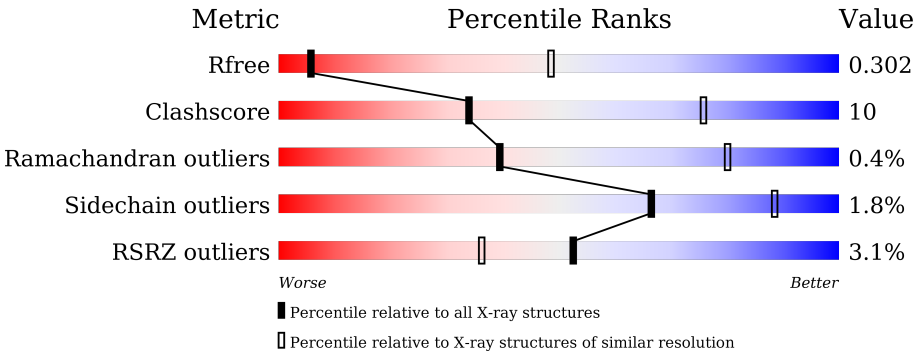
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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	803	2% 79% 17%
1	B	803	2% 73% 22%
1	C	803	3% 77% 18%
1	D	803	4% 80% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	901	-	-	-	X
2	NAG	C	901	-	-	-	X
3	GYK	A	902	-	-	-	X
3	GYK	C	902	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24066 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			5970	3835	990	1116	29			
1	B	773	Total	C	N	O	S	0	0	0
			6001	3850	991	1131	29			
1	C	773	Total	C	N	O	S	0	0	0
			5960	3829	987	1116	28			
1	D	776	Total	C	N	O	S	0	0	0
			5975	3835	991	1121	28			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	?	-	VAL	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	827	GLY	-	cloning artifact	UNP P19491
A	828	LEU	-	cloning artifact	UNP P19491
A	829	VAL	-	cloning artifact	UNP P19491
A	830	PRO	-	cloning artifact	UNP P19491
A	831	ARG	-	cloning artifact	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	?	-	VAL	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491

Continued on next page...

Continued from previous page...

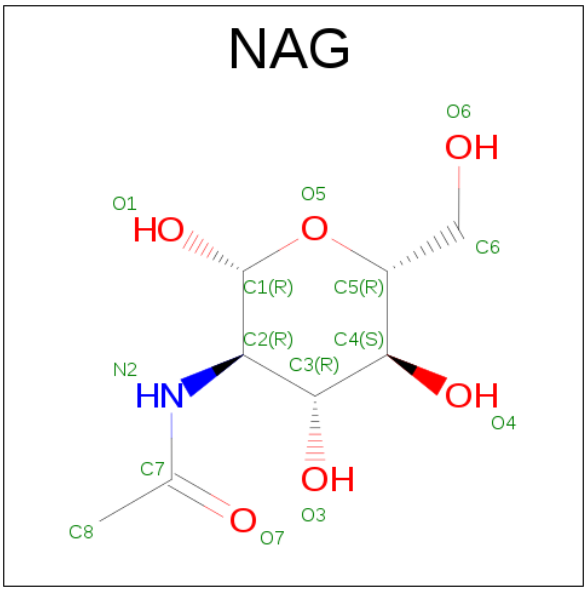
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	827	GLY	-	cloning artifact	UNP P19491
B	828	LEU	-	cloning artifact	UNP P19491
B	829	VAL	-	cloning artifact	UNP P19491
B	830	PRO	-	cloning artifact	UNP P19491
B	831	ARG	-	cloning artifact	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	?	-	VAL	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	827	GLY	-	cloning artifact	UNP P19491
C	828	LEU	-	cloning artifact	UNP P19491
C	829	VAL	-	cloning artifact	UNP P19491
C	830	PRO	-	cloning artifact	UNP P19491
C	831	ARG	-	cloning artifact	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	?	-	VAL	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491

Continued on next page...

Continued from previous page...

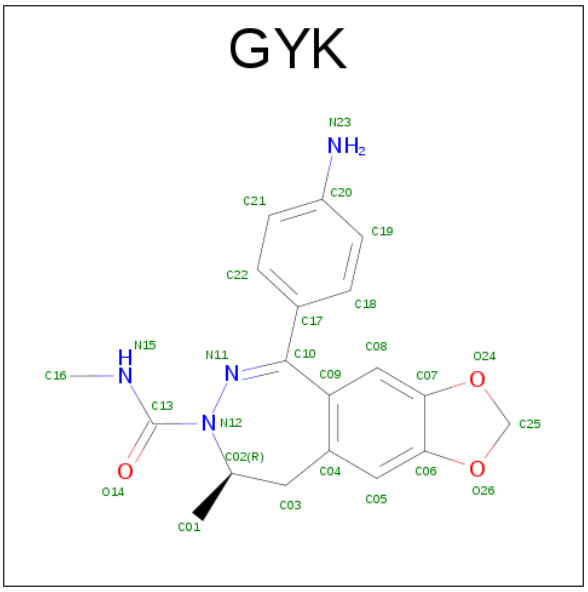
Chain	Residue	Modelled	Actual	Comment	Reference
D	564	ASP	-	linker	UNP P19491
D	565	THR	-	linker	UNP P19491
D	566	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	827	GLY	-	cloning artifact	UNP P19491
D	828	LEU	-	cloning artifact	UNP P19491
D	829	VAL	-	cloning artifact	UNP P19491
D	830	PRO	-	cloning artifact	UNP P19491
D	831	ARG	-	cloning artifact	UNP P19491

- Molecule 2 is 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
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (8R)-5-(4-aminophenyl)-N,8-dimethyl-8,9-dihydro-2H,7H-[1,3]dioxolo[4,5-h][2,3]benzodiazepine-7-carboxamide (three-letter code: GYK) (formula: $C_{19}H_{20}N_4O_3$).



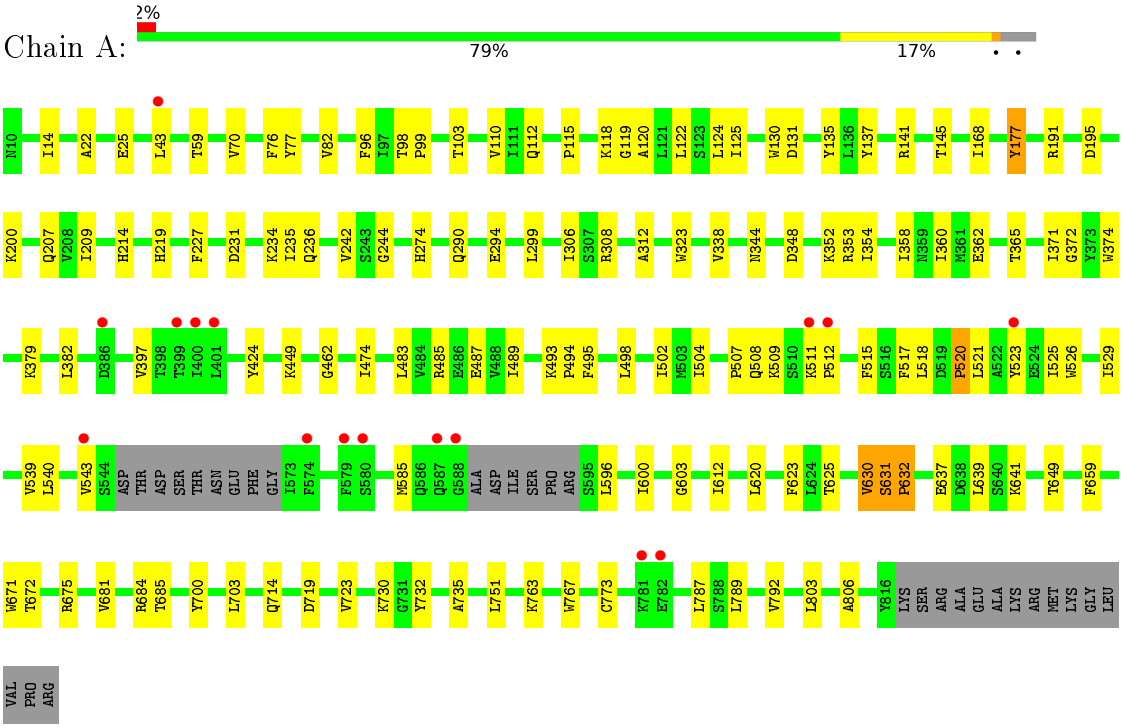
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	19	4	3		
3	B	1	Total	C	N	O	0	0
			26	19	4	3		
3	C	1	Total	C	N	O	0	0
			26	19	4	3		
3	D	1	Total	C	N	O	0	0
			26	19	4	3		

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.

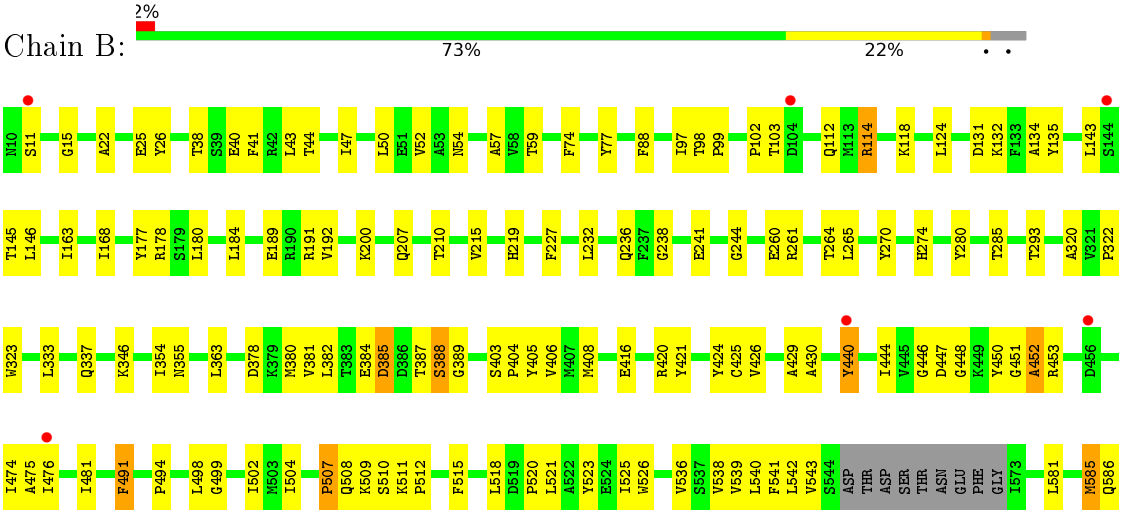
- Molecule 1: Glutamate receptor 2

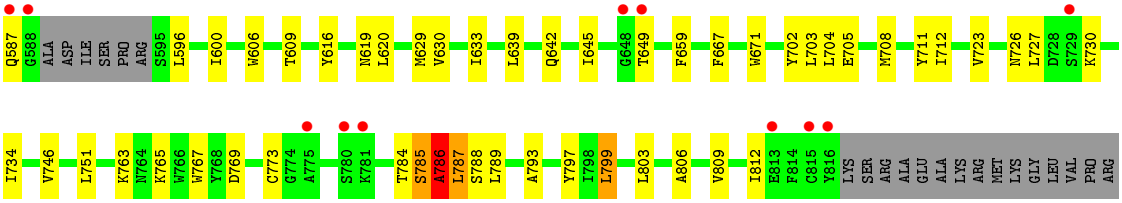
Chain A:



- Molecule 1: Glutamate receptor 2

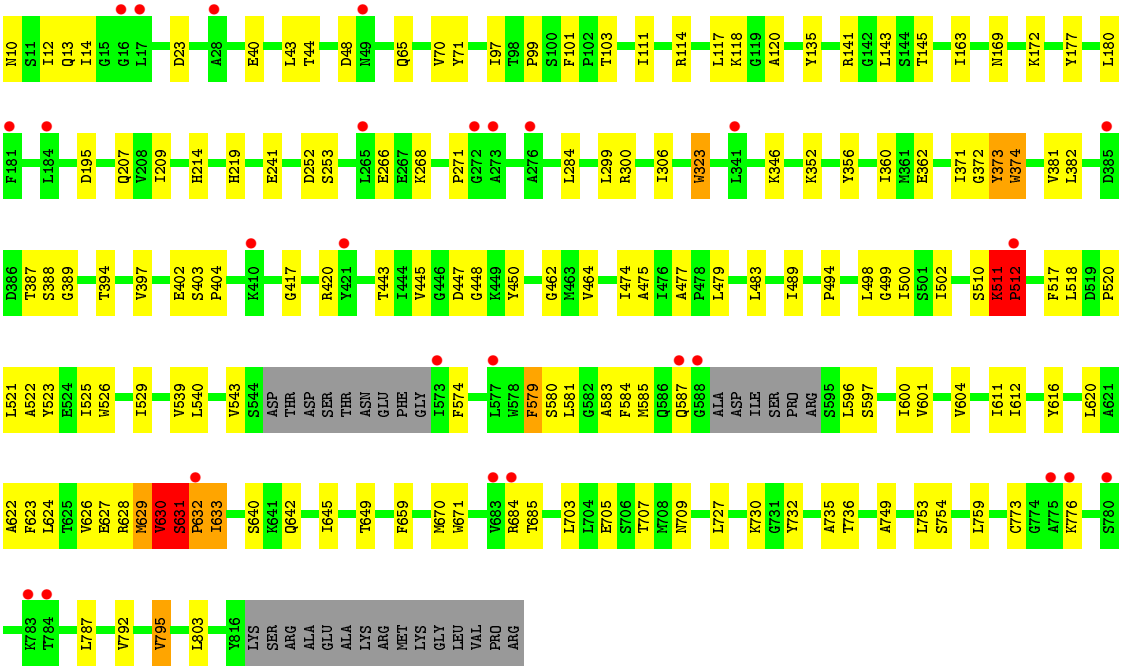
Chain B:





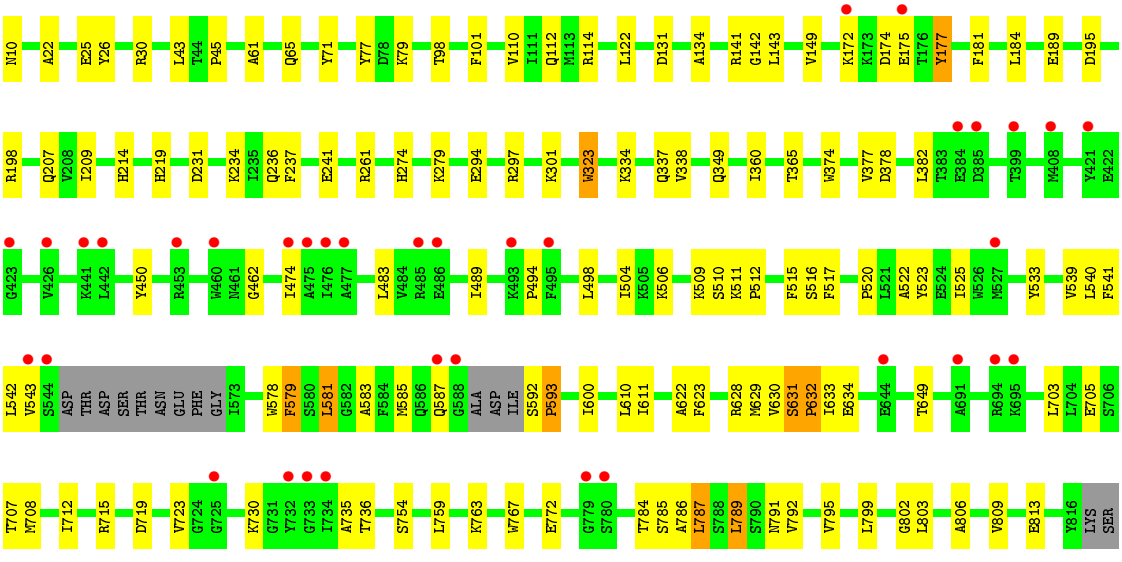
• Molecule 1: Glutamate receptor 2

Chain C:



• Molecule 1: Glutamate receptor 2

Chain D:




ARG
ALA
GLU
ALA
LYS
ARG
MET
LYS
GLY
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.59Å 110.64Å 599.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 3.80 47.49 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.49-3.80) 98.9 (47.49-3.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.276 , 0.292 0.281 , 0.302	Depositor DCC
R_{free} test set	3070 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	141.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 101.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å^2)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GYK, NAG

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	0.27	2/6092 (0.0%)	0.44	1/8244 (0.0%)
1	B	0.27	1/6123 (0.0%)	0.55	8/8284 (0.1%)
1	C	0.27	2/6082 (0.0%)	0.50	6/8235 (0.1%)
1	D	0.29	2/6098 (0.0%)	0.45	4/8257 (0.0%)
All	All	0.28	7/24395 (0.0%)	0.49	19/33020 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	632	PRO	N-CD	9.86	1.61	1.47
1	B	388	SER	N-CA	6.05	1.58	1.46
1	D	512	PRO	N-CD	5.47	1.55	1.47
1	C	632	PRO	N-CD	5.45	1.55	1.47
1	A	632	PRO	N-CD	5.38	1.55	1.47
1	A	512	PRO	N-CD	5.27	1.55	1.47
1	C	512	PRO	N-CD	5.11	1.55	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	452	ALA	CB-CA-C	-14.64	88.14	110.10
1	C	629	MET	CB-CA-C	-12.59	85.22	110.40
1	B	452	ALA	N-CA-C	12.33	144.30	111.00
1	B	785	SER	CB-CA-C	10.37	129.81	110.10
1	B	453	ARG	N-CA-CB	-10.05	92.51	110.60
1	B	786	ALA	N-CA-CB	9.57	123.50	110.10
1	D	632	PRO	CA-N-CD	-8.14	100.10	111.50
1	B	388	SER	N-CA-C	-6.97	92.19	111.00
1	B	388	SER	CB-CA-C	6.92	123.24	110.10
1	D	631	SER	C-N-CD	6.91	142.92	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	512	PRO	CA-N-CD	-6.66	102.17	111.50
1	B	388	SER	N-CA-CB	6.12	119.67	110.50
1	C	373	TYR	CB-CA-C	5.86	122.12	110.40
1	D	631	SER	CB-CA-C	5.76	121.05	110.10
1	A	511	LYS	C-N-CD	5.57	140.10	128.40
1	D	511	LYS	C-N-CD	5.46	139.86	128.40
1	C	630	VAL	N-CA-C	-5.27	96.76	111.00
1	C	511	LYS	C-N-CD	5.10	139.10	128.40
1	C	374	TRP	N-CA-CB	5.05	119.69	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5970	0	5874	124	0
1	B	6001	0	5924	139	1
1	C	5960	0	5850	154	0
1	D	5975	0	5855	109	1
2	A	14	0	13	1	0
2	B	14	0	13	1	0
2	C	14	0	13	1	0
2	D	14	0	13	1	0
3	A	26	0	0	1	0
3	B	26	0	0	3	0
3	C	26	0	0	3	0
3	D	26	0	0	2	0
All	All	24066	0	23555	482	1

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 10.

All (482) 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:D:628:ARG:CB	1:D:630:VAL:HG22	1.12	1.55
1:C:512:PRO:HG3	3:C:902:GYK:C16	1.51	1.40
1:D:628:ARG:CB	1:D:630:VAL:CG2	2.02	1.35
1:A:77:TYR:CD1	1:A:82:VAL:HB	1.65	1.28
1:C:622:ALA:O	1:C:626:VAL:HG23	1.39	1.20
1:D:631:SER:HB3	1:D:632:PRO:HA	1.23	1.14
1:A:77:TYR:CE1	1:A:82:VAL:CG2	2.32	1.12
1:C:630:VAL:HG22	1:C:632:PRO:HA	1.30	1.10
1:A:630:VAL:HA	1:A:631:SER:HB2	1.21	1.06
1:A:77:TYR:CD1	1:A:82:VAL:CB	2.41	1.02
1:C:632:PRO:HD2	1:C:633:ILE:HB	1.38	1.01
1:A:77:TYR:CE1	1:A:82:VAL:HB	1.96	0.99
1:D:377:VAL:HG13	1:D:378:ASP:H	1.26	0.98
1:C:630:VAL:HG22	1:C:631:SER:H	1.29	0.98
1:C:631:SER:H	1:C:632:PRO:HA	1.30	0.97
1:C:521:LEU:HG	1:C:616:TYR:HD2	1.29	0.96
1:C:629:MET:CG	1:C:629:MET:O	2.03	0.95
1:B:232:LEU:O	1:B:232:LEU:HD23	1.66	0.95
1:C:632:PRO:CD	1:C:633:ILE:HB	1.95	0.95
1:C:622:ALA:O	1:C:626:VAL:CG2	2.14	0.95
1:A:449:LYS:HB3	1:A:462:GLY:HA2	1.49	0.94
1:D:623:PHE:HD2	1:D:629:MET:HE3	1.31	0.93
1:A:77:TYR:HD1	1:A:82:VAL:HB	1.30	0.93
1:C:629:MET:HG2	1:C:629:MET:O	1.66	0.92
1:D:631:SER:CB	1:D:632:PRO:HA	2.00	0.91
1:A:77:TYR:CE1	1:A:82:VAL:CB	2.53	0.90
1:A:77:TYR:CE1	1:A:82:VAL:HG23	2.06	0.90
1:A:630:VAL:HG22	1:A:631:SER:C	1.92	0.90
1:A:631:SER:HB3	1:A:632:PRO:HA	1.54	0.90
1:B:541:PHE:HD2	1:B:542:LEU:CD2	1.84	0.90
1:A:630:VAL:HA	1:A:631:SER:CB	2.02	0.88
1:D:623:PHE:HD2	1:D:629:MET:CE	1.86	0.87
1:C:512:PRO:CG	3:C:902:GYK:C16	2.48	0.86
1:B:232:LEU:HD21	1:B:363:LEU:HD22	1.56	0.86
1:B:541:PHE:CD2	1:B:542:LEU:HD23	2.11	0.85
1:B:541:PHE:CD2	1:B:542:LEU:CD2	2.62	0.83
1:C:632:PRO:CB	1:C:633:ILE:HB	2.09	0.82
1:B:382:LEU:HD13	1:B:384:GLU:CG	2.10	0.81
1:C:632:PRO:HB2	1:C:633:ILE:HB	1.60	0.81
1:C:631:SER:N	1:C:632:PRO:HA	1.96	0.80
1:C:632:PRO:HB2	1:C:633:ILE:CG1	2.12	0.80
1:D:377:VAL:HG13	1:D:378:ASP:N	1.95	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:HD2	1:C:633:ILE:CB	2.13	0.79
1:A:77:TYR:CE1	1:A:82:VAL:HG21	2.20	0.76
1:D:623:PHE:CD2	1:D:629:MET:CE	2.69	0.76
1:B:114:ARG:HD2	1:B:280:TYR:HE2	1.51	0.76
1:C:521:LEU:HG	1:C:616:TYR:CD2	2.18	0.76
1:C:632:PRO:HB2	1:C:633:ILE:CB	2.15	0.75
1:B:451:GLY:HA2	1:B:452:ALA:HB3	1.67	0.75
1:B:541:PHE:HD2	1:B:542:LEU:HD21	1.51	0.74
1:D:715:ARG:HD3	1:D:772:GLU:HG2	1.68	0.74
1:B:227:PHE:CZ	1:B:232:LEU:HD11	2.23	0.74
1:C:630:VAL:HG22	1:C:631:SER:N	2.02	0.74
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.68	0.73
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.71	0.72
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.70	0.72
1:A:520:PRO:O	1:B:787:LEU:HD12	1.89	0.72
1:C:630:VAL:HG22	1:C:632:PRO:CA	2.16	0.72
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.72
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:D:377:VAL:CG1	1:D:378:ASP:H	2.01	0.71
1:B:382:LEU:HD13	1:B:384:GLU:HG2	1.73	0.70
1:C:632:PRO:HB2	1:C:633:ILE:HG13	1.73	0.70
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.74	0.69
1:D:198:ARG:HH21	1:D:279:LYS:HD3	1.58	0.68
1:D:509:LYS:HA	1:D:510:SER:C	2.13	0.68
1:A:77:TYR:CZ	1:A:82:VAL:HG23	2.28	0.68
1:C:631:SER:OG	1:C:632:PRO:O	2.10	0.68
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.76	0.68
1:B:382:LEU:HD13	1:B:384:GLU:HG3	1.75	0.67
1:A:603:GLY:HA2	1:B:585:MET:HB3	1.76	0.67
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.59	0.67
1:C:640:SER:HB3	1:C:670:MET:HG2	1.77	0.67
1:C:522:ALA:HB3	1:C:525:ILE:HD13	1.76	0.67
1:A:539:VAL:HG21	1:B:803:LEU:HD22	1.77	0.66
1:A:70:VAL:O	1:A:308:ARG:NH1	2.29	0.66
1:C:371:ILE:O	1:C:382:LEU:HD22	1.95	0.66
1:D:623:PHE:CD2	1:D:629:MET:HE2	2.30	0.66
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.61	0.66
1:D:631:SER:HB3	1:D:632:PRO:CA	2.15	0.65
1:C:596:LEU:HD13	1:D:578:TRP:HA	1.79	0.65
1:B:388:SER:HB3	1:B:389:GLY:HA3	1.77	0.64
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:HIS:O	1:A:274:HIS:ND1	2.30	0.64
1:A:630:VAL:HG13	1:A:631:SER:O	1.97	0.64
1:D:630:VAL:O	1:D:630:VAL:HG12	1.97	0.64
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.80	0.64
1:A:344:ASN:ND2	2:A:901:NAG:O6	2.31	0.64
1:B:385:ASP:OD2	1:B:385:ASP:N	2.29	0.64
1:B:541:PHE:CD2	1:B:542:LEU:HD21	2.31	0.64
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.31	0.64
1:D:377:VAL:HG13	1:D:378:ASP:OD1	1.98	0.63
1:C:498:LEU:HD21	1:C:732:TYR:CZ	2.33	0.63
1:A:630:VAL:HG22	1:A:631:SER:O	1.98	0.63
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.64	0.63
1:A:110:VAL:CG1	1:A:112:GLN:NE2	2.61	0.63
1:B:103:THR:HG23	1:B:112:GLN:HE21	1.64	0.62
1:C:587:GLN:HE22	1:D:587:GLN:HG3	1.64	0.62
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.81	0.62
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.80	0.62
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.81	0.62
1:A:529:ILE:HD13	1:A:612:ILE:HD12	1.81	0.62
1:C:511:LYS:H	1:C:512:PRO:HD2	1.64	0.61
1:C:626:VAL:O	1:C:629:MET:HB3	2.00	0.61
1:C:630:VAL:CG2	1:C:631:SER:H	2.11	0.61
1:C:346:LYS:NZ	2:C:901:NAG:O7	2.34	0.60
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.84	0.60
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.67	0.60
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.84	0.60
1:D:628:ARG:CB	1:D:629:MET:HA	2.32	0.60
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.82	0.59
1:A:623:PHE:HZ	1:B:786:ALA:O	1.85	0.59
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.84	0.59
1:C:623:PHE:HZ	1:D:786:ALA:HA	1.67	0.59
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.85	0.59
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.35	0.59
1:B:498:LEU:HD12	1:B:705:GLU:HB2	1.83	0.59
1:D:516:SER:HB2	3:D:902:GYK:C01	2.33	0.59
1:C:521:LEU:HB2	1:C:526:TRP:CE2	2.38	0.58
1:A:681:VAL:O	1:A:700:TYR:OH	2.20	0.58
1:A:493:LYS:HG3	1:A:751:LEU:HD21	1.86	0.58
1:B:447:ASP:N	1:B:448:GLY:HA2	2.18	0.58
1:C:143:LEU:HG	1:D:143:LEU:HD11	1.85	0.58
1:C:773:CYS:HB3	1:C:776:LYS:CB	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:PRO:CG	1:C:633:ILE:HB	2.33	0.58
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.86	0.58
1:B:508:GLN:N	1:B:509:LYS:HA	2.19	0.58
1:A:792:VAL:HG21	1:D:525:ILE:HG12	1.85	0.58
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.33	0.58
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.86	0.58
1:C:518:LEU:O	1:C:526:TRP:NE1	2.36	0.58
1:A:630:VAL:CA	1:A:631:SER:HB2	2.14	0.57
1:C:498:LEU:HD12	1:C:730:LYS:HG3	1.85	0.57
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.84	0.57
1:A:374:TRP:CE3	1:A:379:LYS:NZ	2.70	0.57
1:A:498:LEU:HD12	1:A:730:LYS:HG3	1.87	0.57
1:A:520:PRO:HG3	1:A:620:LEU:HD13	1.87	0.57
1:A:684:ARG:HG2	1:A:685:THR:HG23	1.87	0.56
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.23	0.56
1:A:344:ASN:O	1:A:353:ARG:NH2	2.38	0.56
1:A:631:SER:CB	1:A:632:PRO:HA	2.33	0.56
1:B:102:PRO:HA	1:B:112:GLN:HG2	1.87	0.56
1:C:597:SER:N	1:D:813:GLU:OE2	2.39	0.56
1:B:620:LEU:HD11	3:B:902:GYK:C18	2.35	0.56
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.88	0.56
1:D:219:HIS:HA	1:D:241:GLU:O	2.06	0.56
1:C:450:TYR:O	1:C:462:GLY:HA3	2.06	0.56
1:B:134:ALA:HB3	1:B:192:VAL:HG22	1.88	0.56
1:B:50:LEU:C	1:B:50:LEU:HD12	2.26	0.56
1:C:522:ALA:H	1:D:787:LEU:HD12	1.71	0.56
1:B:784:THR:O	1:B:785:SER:OG	2.22	0.56
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.87	0.56
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.87	0.55
1:C:445:VAL:HG22	1:C:448:GLY:H	1.72	0.55
1:C:13:GLN:HA	1:C:44:THR:HB	1.89	0.55
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.40	0.55
1:B:232:LEU:CD2	1:B:363:LEU:HD22	2.33	0.55
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.88	0.55
1:A:135:TYR:CE1	1:A:137:TYR:HB3	2.41	0.55
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.70	0.55
1:B:538:VAL:O	1:B:541:PHE:HB3	2.07	0.54
1:C:371:ILE:HA	1:C:382:LEU:HD22	1.89	0.54
1:C:510:SER:CB	1:C:511:LYS:CA	2.85	0.54
1:C:510:SER:CB	1:C:511:LYS:CB	2.85	0.54
1:B:38:THR:HG23	1:B:40:GLU:H	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.90	0.54
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.90	0.54
1:D:623:PHE:CD2	1:D:629:MET:HE3	2.24	0.54
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.73	0.54
1:B:799:LEU:O	1:B:803:LEU:N	2.39	0.54
1:D:334:LYS:NZ	1:D:349:GLN:O	2.27	0.54
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.41	0.54
1:A:751:LEU:HB2	1:D:483:LEU:HD13	1.89	0.54
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.88	0.54
1:A:517:PHE:HE1	1:D:611:ILE:HG21	1.73	0.54
1:A:77:TYR:CD1	1:A:82:VAL:CG2	2.83	0.53
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.38	0.53
1:A:714:GLN:HA	1:A:773:CYS:HB2	1.91	0.53
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.91	0.53
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.89	0.53
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.90	0.53
1:C:539:VAL:HG21	1:D:803:LEU:HD22	1.91	0.53
1:A:77:TYR:CZ	1:A:82:VAL:CG2	2.88	0.53
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.44	0.53
1:A:141:ARG:NH2	1:A:195:ASP:O	2.33	0.53
1:B:236:GLN:HG3	1:B:363:LEU:HD11	1.90	0.53
1:B:600:ILE:HG22	1:C:581:LEU:HD13	1.91	0.53
1:B:114:ARG:HD2	1:B:280:TYR:CE2	2.38	0.52
1:D:509:LYS:N	1:D:510:SER:CB	2.72	0.52
1:B:596:LEU:HB2	1:C:574:PHE:O	2.09	0.52
1:C:596:LEU:HG	1:D:809:VAL:HG11	1.91	0.52
1:B:620:LEU:HD11	3:B:902:GYK:C19	2.39	0.52
1:B:504:ILE:HD13	1:B:633:ILE:HD12	1.91	0.52
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.91	0.52
1:A:119:GLY:O	1:A:379:LYS:NZ	2.41	0.52
1:B:163:ILE:HG21	1:B:180:LEU:HD13	1.92	0.52
1:D:22:ALA:HB1	1:D:25:GLU:HB2	1.90	0.52
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.91	0.52
1:B:606:TRP:HA	1:B:609:THR:HG22	1.91	0.52
1:B:510:SER:OG	3:B:902:GYK:O14	2.27	0.51
1:B:784:THR:C	1:B:785:SER:OG	2.49	0.51
1:B:510:SER:HB3	1:B:512:PRO:HD3	1.92	0.51
1:C:394:THR:HG23	1:C:394:THR:O	2.10	0.51
1:D:784:THR:HA	1:D:785:SER:HB3	1.92	0.51
1:B:787:LEU:HD23	1:B:788:SER:N	2.24	0.51
1:D:541:PHE:HD2	1:D:542:LEU:HD23	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD21	1:B:293:THR:HG22	1.93	0.51
1:B:659:PHE:HB3	1:B:671:TRP:HB2	1.93	0.51
1:C:511:LYS:H	1:C:512:PRO:CD	2.24	0.51
1:B:26:TYR:HE1	1:B:47:ILE:HG12	1.75	0.51
1:C:97:ILE:HA	1:C:111:ILE:HB	1.93	0.51
1:C:604:VAL:HG12	1:D:799:LEU:HD12	1.92	0.51
1:C:477:ALA:O	1:C:479:LEU:N	2.42	0.51
1:D:517:PHE:CE1	1:D:795:VAL:HG22	2.46	0.51
1:A:803:LEU:HD22	1:D:539:VAL:HG21	1.93	0.51
1:B:177:TYR:HB3	1:B:207:GLN:HG2	1.92	0.50
1:C:498:LEU:CD1	1:C:730:LYS:CD	2.88	0.50
1:A:631:SER:HB3	1:A:632:PRO:CA	2.34	0.50
1:C:498:LEU:HD12	1:C:499:GLY:N	2.26	0.50
1:A:502:ILE:HD13	1:A:639:LEU:HD13	1.92	0.50
1:A:525:ILE:HG13	1:B:789:LEU:HD12	1.92	0.50
1:B:15:GLY:O	1:B:74:PHE:N	2.40	0.50
1:C:500:ILE:O	1:C:727:LEU:N	2.44	0.50
1:A:103:THR:O	1:A:352:LYS:NZ	2.43	0.50
1:B:232:LEU:O	1:B:232:LEU:CD2	2.50	0.50
1:B:508:GLN:H	1:B:509:LYS:HA	1.77	0.50
1:A:77:TYR:CD1	1:A:82:VAL:CA	2.94	0.50
1:B:131:ASP:OD1	1:B:132:LYS:N	2.45	0.50
1:C:252:ASP:OD1	1:C:253:SER:N	2.45	0.49
1:C:10:ASN:ND2	1:C:40:GLU:O	2.45	0.49
1:D:209:ILE:HA	1:D:214:HIS:CD2	2.46	0.49
1:D:382:LEU:H	1:D:382:LEU:HD23	1.76	0.49
1:B:168:ILE:HD11	1:B:200:LYS:HZ3	1.77	0.49
1:A:96:PHE:CE2	1:A:98:THR:HB	2.48	0.49
1:B:124:LEU:HA	1:B:380:MET:HE1	1.93	0.49
1:C:579:PHE:O	1:C:583:ALA:N	2.46	0.49
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.47	0.49
1:C:525:ILE:HD11	1:D:789:LEU:HA	1.94	0.49
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.94	0.49
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.76	0.49
1:B:11:SER:OG	1:B:44:THR:OG1	2.27	0.49
1:B:510:SER:HB3	1:B:511:LYS:HA	1.94	0.49
1:A:623:PHE:CZ	1:B:786:ALA:N	2.81	0.49
1:C:371:ILE:C	1:C:382:LEU:HD22	2.32	0.49
1:D:628:ARG:N	1:D:629:MET:HB2	2.28	0.49
1:A:177:TYR:HD2	1:A:207:GLN:HG3	1.77	0.49
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:LYS:N	1:D:719:ASP:O	2.40	0.49
1:C:498:LEU:HB3	1:C:707:THR:HG23	1.94	0.49
1:A:308:ARG:NE	1:A:312:ALA:HB2	2.28	0.49
1:C:373:TYR:HB3	1:C:381:VAL:O	2.13	0.49
1:C:604:VAL:HG11	1:D:802:GLY:HA3	1.95	0.49
1:B:50:LEU:CD1	1:B:52:VAL:HA	2.43	0.48
1:D:708:MET:O	1:D:712:ILE:HG12	2.14	0.48
1:B:525:ILE:HG12	1:C:792:VAL:HG11	1.94	0.48
1:D:26:TYR:CE2	1:D:30:ARG:HD2	2.48	0.48
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.95	0.48
1:B:387:THR:OG1	1:B:387:THR:O	2.31	0.48
1:B:184:LEU:O	1:B:189:GLU:HB2	2.13	0.48
3:D:902:GYK:C08	3:D:902:GYK:C22	2.92	0.48
1:A:22:ALA:HB1	1:A:25:GLU:HB2	1.94	0.48
1:B:381:VAL:O	1:B:381:VAL:HG13	2.14	0.48
1:C:219:HIS:HA	1:C:241:GLU:O	2.14	0.48
1:A:498:LEU:HD21	1:A:732:TYR:CZ	2.49	0.48
1:A:637:GLU:O	1:A:641:LYS:N	2.47	0.47
1:B:210:THR:HG22	1:D:237:PHE:HB2	1.96	0.47
1:C:135:TYR:HH	1:C:145:THR:HG1	1.57	0.47
1:C:498:LEU:HD12	1:C:730:LYS:CG	2.43	0.47
1:A:789:LEU:HA	1:D:525:ILE:HD11	1.96	0.47
1:D:236:GLN:NE2	1:D:365:THR:O	2.39	0.47
1:B:227:PHE:CZ	1:B:232:LEU:CD1	2.95	0.47
1:B:97:ILE:HD11	1:B:333:LEU:HD22	1.96	0.47
1:C:388:SER:H	1:C:389:GLY:HA2	1.80	0.47
1:D:377:VAL:CG1	1:D:378:ASP:N	2.65	0.47
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.97	0.47
1:D:630:VAL:CG1	1:D:630:VAL:O	2.62	0.47
1:A:596:LEU:HA	1:A:596:LEU:HD12	1.84	0.47
1:A:623:PHE:CZ	1:B:786:ALA:O	2.67	0.47
1:D:174:ASP:OD1	1:D:207:GLN:NE2	2.48	0.47
1:D:763:LYS:O	1:D:767:TRP:HB2	2.15	0.47
1:B:630:VAL:HG23	1:B:630:VAL:O	2.15	0.47
1:C:632:PRO:HD2	1:C:633:ILE:CG2	2.44	0.47
1:B:405:TYR:HB3	1:B:425:CYS:SG	2.55	0.46
1:A:110:VAL:HG12	1:A:112:GLN:NE2	2.30	0.46
1:B:425:CYS:O	1:B:429:ALA:N	2.49	0.46
1:B:99:PRO:O	1:B:114:ARG:HB2	2.15	0.46
1:C:510:SER:CB	1:C:511:LYS:HA	2.46	0.46
1:B:444:ILE:HG22	1:B:446:GLY:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LEU:HD12	1:C:730:LYS:HD2	1.98	0.46
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.31	0.46
1:C:498:LEU:CD2	1:C:732:TYR:CZ	2.98	0.46
1:B:499:GLY:HA3	1:B:726:ASN:HB3	1.97	0.46
1:B:708:MET:O	1:B:712:ILE:HG12	2.15	0.46
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.98	0.46
1:D:131:ASP:N	1:D:131:ASP:OD1	2.47	0.46
1:B:22:ALA:HB1	1:B:25:GLU:HB2	1.97	0.46
1:C:387:THR:HA	1:C:388:SER:HA	1.62	0.46
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.97	0.46
1:A:274:HIS:O	1:A:274:HIS:CG	2.69	0.46
1:C:371:ILE:HA	1:C:382:LEU:CD2	2.44	0.46
1:C:447:ASP:OD1	1:C:447:ASP:N	2.44	0.46
1:D:715:ARG:HA	1:D:772:GLU:CG	2.46	0.46
1:C:371:ILE:CA	1:C:382:LEU:HD22	2.44	0.46
1:D:787:LEU:HD11	1:D:792:VAL:HG21	1.97	0.46
1:C:600:ILE:HD11	1:D:806:ALA:HA	1.98	0.46
1:D:632:PRO:O	1:D:632:PRO:HD2	2.16	0.45
1:A:521:LEU:HB2	1:A:526:TRP:NE1	2.31	0.45
1:C:520:PRO:HG3	1:C:620:LEU:HD13	1.98	0.45
1:B:809:VAL:O	1:B:812:ILE:HG12	2.16	0.45
1:D:623:PHE:CE2	1:D:629:MET:HE2	2.52	0.45
1:A:507:PRO:HA	1:A:508:GLN:CB	2.47	0.45
1:A:507:PRO:HB2	1:A:509:LYS:CB	2.45	0.45
1:B:515:PHE:CG	1:B:515:PHE:O	2.69	0.45
1:B:587:GLN:HB3	1:B:606:TRP:CD1	2.51	0.45
1:C:177:TYR:CB	1:C:207:GLN:HG2	2.45	0.45
1:C:464:VAL:HG22	1:C:479:LEU:HD21	1.99	0.45
1:D:181:PHE:HA	1:D:184:LEU:HB2	1.98	0.45
1:A:424:TYR:HE2	1:A:495:PHE:HE2	1.65	0.45
1:B:38:THR:HG23	1:B:41:PHE:H	1.81	0.45
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.99	0.45
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.81	0.45
1:C:521:LEU:HA	1:D:787:LEU:HG	1.98	0.45
1:C:631:SER:CB	1:C:632:PRO:C	2.85	0.45
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.99	0.45
1:D:143:LEU:HD23	1:D:143:LEU:H	1.80	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.99	0.45
1:B:498:LEU:HG	1:B:730:LYS:HG3	1.99	0.45
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.98	0.45
1:B:751:LEU:HB2	1:C:483:LEU:HD13	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:LYS:CA	1:D:510:SER:C	2.85	0.45
1:D:541:PHE:CD2	1:D:542:LEU:HD23	2.51	0.45
1:A:630:VAL:CA	1:A:631:SER:CB	2.85	0.44
1:B:232:LEU:HD21	1:B:363:LEU:CD2	2.37	0.44
1:C:464:VAL:HG13	1:C:489:ILE:HG12	1.98	0.44
1:D:592:SER:N	1:D:593:PRO:HD3	2.31	0.44
1:A:397:VAL:HG13	1:A:474:ILE:HG23	1.99	0.44
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.81	0.44
1:A:787:LEU:O	1:D:522:ALA:HB2	2.16	0.44
1:A:235:ILE:HD12	1:A:242:VAL:HG21	1.99	0.44
1:A:485:ARG:O	1:A:489:ILE:HG13	2.17	0.44
1:A:631:SER:HA	1:A:632:PRO:C	2.37	0.44
1:B:406:VAL:HG22	1:B:426:VAL:HG23	1.99	0.44
1:A:115:PRO:HA	1:A:353:ARG:HB2	1.99	0.44
1:B:260:GLU:O	1:B:264:THR:OG1	2.27	0.44
1:B:404:PRO:HG3	1:B:711:TYR:CD1	2.52	0.44
1:A:498:LEU:HD12	1:A:730:LYS:CG	2.47	0.44
1:C:498:LEU:HD11	1:C:730:LYS:CD	2.48	0.44
3:C:902:GYK:C22	3:C:902:GYK:C08	2.95	0.44
1:D:632:PRO:O	1:D:633:ILE:C	2.56	0.44
1:A:449:LYS:CB	1:A:462:GLY:HA2	2.35	0.44
1:A:620:LEU:HD11	3:A:902:GYK:C18	2.48	0.44
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.99	0.44
1:D:297:ARG:HG2	1:D:301:LYS:HE3	2.00	0.44
1:D:754:SER:HB2	1:D:759:LEU:HD12	2.00	0.44
1:C:611:ILE:HB	1:D:795:VAL:HG11	1.98	0.44
1:B:430:ALA:HA	1:B:440:TYR:HE1	1.83	0.44
1:B:54:ASN:OD1	1:B:57:ALA:N	2.48	0.44
1:A:520:PRO:C	1:B:787:LEU:HD12	2.38	0.44
1:B:787:LEU:CD2	1:B:788:SER:N	2.80	0.44
1:A:540:LEU:HA	1:A:543:VAL:HG22	1.99	0.44
1:C:521:LEU:HB2	1:C:526:TRP:NE1	2.33	0.44
1:A:236:GLN:NE2	1:A:365:THR:O	2.49	0.44
1:A:59:THR:HG21	1:B:59:THR:HG21	2.00	0.44
1:B:11:SER:HG	1:B:44:THR:HG1	1.64	0.44
1:B:539:VAL:HG21	1:C:803:LEU:HD22	1.99	0.44
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.00	0.43
1:D:579:PHE:O	1:D:583:ALA:N	2.50	0.43
1:A:14:ILE:HD13	1:A:43:LEU:HD23	2.00	0.43
1:A:623:PHE:HZ	1:B:786:ALA:N	2.15	0.43
1:A:130:TRP:HZ2	1:A:219:HIS:CD2	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:TYR:CE1	1:B:47:ILE:HG12	2.54	0.43
1:A:504:ILE:HD11	1:A:723:VAL:HG11	2.00	0.43
1:C:163:ILE:HG21	1:C:180:LEU:HD13	1.98	0.43
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.54	0.43
1:D:141:ARG:NH2	1:D:195:ASP:OD1	2.50	0.43
1:A:76:PHE:CE2	1:A:99:PRO:HG2	2.54	0.43
1:B:787:LEU:CD2	1:B:787:LEU:C	2.86	0.43
1:C:209:ILE:HG23	1:C:214:HIS:CE1	2.54	0.43
1:D:504:ILE:HD11	1:D:723:VAL:HG11	2.00	0.43
1:B:481:ILE:HG23	1:B:491:PHE:CD2	2.54	0.43
1:C:627:GLU:O	1:C:629:MET:N	2.52	0.43
1:A:372:GLY:HA2	1:A:382:LEU:HB3	2.00	0.43
1:B:763:LYS:O	1:B:767:TRP:HB2	2.18	0.43
1:B:168:ILE:HD11	1:B:200:LYS:NZ	2.34	0.43
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.53	0.43
1:B:476:ILE:HG22	1:B:734:ILE:HG23	2.00	0.43
1:D:177:TYR:HD1	1:D:177:TYR:HA	1.73	0.43
1:D:634:GLU:HA	1:D:723:VAL:HB	2.00	0.43
1:A:521:LEU:HA	1:B:787:LEU:HD11	1.16	0.43
1:C:397:VAL:O	1:C:443:THR:OG1	2.30	0.43
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.53	0.43
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.54	0.43
1:C:502:ILE:O	1:C:709:ASN:ND2	2.48	0.43
1:A:118:LYS:HG2	1:A:145:THR:HG22	2.00	0.42
1:C:403:SER:HA	1:C:404:PRO:HA	1.83	0.42
1:C:629:MET:SD	1:C:629:MET:O	2.75	0.42
1:C:498:LEU:HD12	1:C:730:LYS:CD	2.48	0.42
1:C:600:ILE:HG22	1:D:581:LEU:HD13	1.99	0.42
1:A:290:GLN:HG2	1:A:338:VAL:HG21	2.00	0.42
1:B:507:PRO:HD2	1:B:508:GLN:HA	2.01	0.42
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.55	0.42
1:B:408:MET:HG2	1:B:421:TYR:CE1	2.53	0.42
1:C:103:THR:O	1:C:352:LYS:NZ	2.52	0.42
1:C:580:SER:O	1:C:584:PHE:N	2.51	0.42
1:B:619:ASN:HA	1:C:624:LEU:HD13	2.01	0.42
1:D:261:ARG:HA	1:D:261:ARG:HD2	1.83	0.42
1:A:763:LYS:O	1:A:767:TRP:HB2	2.20	0.42
1:C:597:SER:O	1:C:601:VAL:HG23	2.18	0.42
1:C:749:ALA:O	1:C:753:LEU:HG	2.19	0.42
1:A:110:VAL:HG11	1:A:112:GLN:NE2	2.32	0.42
1:A:498:LEU:C	1:A:498:LEU:HD12	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HA	1:A:195:ASP:HB3	2.02	0.42
1:A:362:GLU:HG3	1:A:371:ILE:HG21	2.02	0.42
1:C:498:LEU:CD1	1:C:730:LYS:HG3	2.50	0.42
1:D:474:ILE:HG13	1:D:736:THR:HG22	2.00	0.42
1:A:518:LEU:O	1:A:526:TRP:NE1	2.53	0.42
1:A:719:ASP:OD1	1:A:719:ASP:N	2.52	0.42
1:C:13:GLN:HG2	1:C:70:VAL:HG12	2.01	0.42
1:D:274:HIS:O	1:D:274:HIS:CG	2.72	0.42
1:D:43:LEU:O	1:D:45:PRO:HD3	2.20	0.42
1:B:507:PRO:N	1:B:508:GLN:HA	2.34	0.42
1:C:520:PRO:HB2	1:C:616:TYR:CE2	2.54	0.42
1:A:358:ILE:HB	1:A:374:TRP:CD1	2.54	0.42
1:A:483:LEU:O	1:A:487:GLU:HG3	2.20	0.42
1:C:611:ILE:HG21	1:D:517:PHE:HE1	1.84	0.42
1:D:122:LEU:HD21	1:D:149:VAL:HA	2.00	0.42
1:C:362:GLU:HG3	1:C:371:ILE:HG21	2.01	0.41
1:C:498:LEU:CD2	1:C:732:TYR:CE2	3.03	0.41
1:A:130:TRP:CZ3	1:A:191:ARG:HB3	2.55	0.41
1:D:79:LYS:HD2	1:D:142:GLY:HA2	2.02	0.41
1:C:356:TYR:HH	1:C:374:TRP:HZ3	1.68	0.41
1:C:388:SER:N	1:C:389:GLY:HA2	2.35	0.41
1:C:659:PHE:HB3	1:C:671:TRP:HB2	2.02	0.41
1:A:625:THR:HG22	1:D:622:ALA:HA	2.02	0.41
1:A:168:ILE:HD11	1:A:200:LYS:NZ	2.34	0.41
1:B:265:LEU:HD13	1:B:270:TYR:CD2	2.56	0.41
1:C:266:GLU:HG2	1:C:268:LYS:H	1.85	0.41
1:D:61:ALA:O	1:D:65:GLN:HG2	2.20	0.41
1:D:489:ILE:HD13	1:D:735:ALA:HB1	2.03	0.41
1:B:337:GLN:NE2	2:B:901:NAG:O7	2.53	0.41
1:C:623:PHE:HA	1:C:626:VAL:HG23	2.02	0.41
1:B:793:ALA:HB1	1:B:797:TYR:CE2	2.55	0.41
1:C:71:TYR:HA	1:C:323:TRP:HH2	1.85	0.41
1:C:529:ILE:HD13	1:C:612:ILE:HD12	2.02	0.41
1:D:234:LYS:HG2	1:D:234:LYS:H	1.66	0.41
1:A:77:TYR:CD1	1:A:82:VAL:HA	2.55	0.41
1:A:77:TYR:CD1	1:A:82:VAL:HG23	2.50	0.41
1:B:518:LEU:O	1:B:526:TRP:NE1	2.52	0.41
1:C:475:ALA:HB3	1:C:735:ALA:HB3	2.02	0.41
1:B:320:ALA:O	1:B:322:PRO:HD3	2.20	0.41
1:B:521:LEU:HB2	1:B:526:TRP:CE2	2.56	0.41
1:A:517:PHE:O	1:A:520:PRO:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:CD2	1:B:146:LEU:HD13	2.56	0.41
1:A:600:ILE:HD11	1:B:806:ALA:HA	2.03	0.41
1:C:417:GLY:O	1:C:420:ARG:NE	2.53	0.41
1:C:631:SER:N	1:C:632:PRO:CA	2.77	0.41
1:D:377:VAL:CG1	1:D:378:ASP:OD1	2.68	0.41
1:B:215:VAL:HA	1:B:238:GLY:O	2.21	0.41
1:C:177:TYR:HA	1:C:177:TYR:HD1	1.78	0.41
1:C:684:ARG:HG2	1:C:685:THR:HG23	2.02	0.41
1:D:110:VAL:HG12	1:D:112:GLN:HG3	2.02	0.41
1:D:498:LEU:HG	1:D:730:LYS:HG3	2.03	0.41
1:B:74:PHE:HA	1:B:97:ILE:O	2.21	0.41
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.56	0.41
1:C:631:SER:HB2	1:C:632:PRO:C	2.41	0.41
1:A:348:ASP:HB3	1:A:354:ILE:HG21	2.02	0.40
1:B:261:ARG:O	1:B:265:LEU:HG	2.21	0.40
1:B:346:LYS:HE3	1:B:355:ASN:HD22	1.87	0.40
1:B:474:ILE:HG12	1:B:475:ALA:H	1.85	0.40
1:B:219:HIS:HD2	1:B:241:GLU:O	2.05	0.40
1:B:507:PRO:CD	1:B:508:GLN:HA	2.51	0.40
1:C:447:ASP:OD2	1:C:462:GLY:N	2.53	0.40
1:C:627:GLU:C	1:C:629:MET:N	2.75	0.40
1:A:131:ASP:N	1:A:131:ASP:OD1	2.55	0.40
1:B:502:ILE:HB	1:B:723:VAL:HG23	2.04	0.40
1:C:705:GLU:OE1	1:C:705:GLU:N	2.52	0.40
1:D:715:ARG:HA	1:D:772:GLU:HG2	2.02	0.40
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.94	0.40
1:A:672:THR:HG22	1:A:675:ARG:NH2	2.37	0.40
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.57	0.40
1:B:403:SER:HA	1:B:404:PRO:HA	1.86	0.40
1:D:360:ILE:HD11	1:D:374:TRP:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:ASP:O	1:D:10:ASN:N[1_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	767/803 (96%)	720 (94%)	45 (6%)	2 (0%)	46	83
1	B	767/803 (96%)	713 (93%)	51 (7%)	3 (0%)	39	80
1	C	767/803 (96%)	716 (93%)	45 (6%)	6 (1%)	24	70
1	D	770/803 (96%)	718 (93%)	50 (6%)	2 (0%)	46	83
All	All	3071/3212 (96%)	2867 (93%)	191 (6%)	13 (0%)	39	80

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	786	ALA
1	C	511	LYS
1	C	512	PRO
1	C	628	ARG
1	D	593	PRO
1	D	520	PRO
1	A	520	PRO
1	B	520	PRO
1	A	631	SER
1	C	633	ILE
1	C	631	SER
1	C	630	VAL
1	B	507	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	627/683 (92%)	621 (99%)	6 (1%)	82 92
1	B	638/683 (93%)	618 (97%)	20 (3%)	47 80
1	C	624/683 (91%)	617 (99%)	7 (1%)	80 92
1	D	625/683 (92%)	613 (98%)	12 (2%)	65 87
All	All	2514/2732 (92%)	2469 (98%)	45 (2%)	66 88

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	323	TRP
1	A	515	PHE
1	A	523	TYR
1	A	585	MET
1	A	630	VAL
1	B	88	PHE
1	B	114	ARG
1	B	143	LEU
1	B	178	ARG
1	B	191	ARG
1	B	274	HIS
1	B	323	TRP
1	B	385	ASP
1	B	440	TYR
1	B	450	TYR
1	B	491	PHE
1	B	523	TYR
1	B	581	LEU
1	B	585	MET
1	B	586	GLN
1	B	629	MET
1	B	639	LEU
1	B	773	CYS
1	B	787	LEU
1	B	799	LEU
1	C	323	TRP
1	C	523	TYR
1	C	579	PHE
1	C	585	MET
1	C	631	SER
1	C	787	LEU
1	C	795	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	177	TYR
1	D	323	TRP
1	D	515	PHE
1	D	523	TYR
1	D	533	TYR
1	D	579	PHE
1	D	581	LEU
1	D	585	MET
1	D	610	LEU
1	D	787	LEU
1	D	789	LEU
1	D	791	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	B	112	GLN
1	B	219	HIS
1	C	219	HIS
1	C	587	GLN
1	D	791	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

8 ligands 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	NAG	A	901	1	14,14,15	0.48	0	15,19,21	0.47	0
3	GYK	A	902	-	25,29,29	2.92	9 (36%)	34,42,42	3.00	14 (41%)
2	NAG	B	901	1	14,14,15	0.33	0	15,19,21	0.46	0
3	GYK	B	902	-	25,29,29	2.97	8 (32%)	34,42,42	2.99	11 (32%)
2	NAG	C	901	1	14,14,15	0.28	0	15,19,21	0.53	0
3	GYK	C	902	-	25,29,29	2.89	9 (36%)	34,42,42	3.31	13 (38%)
2	NAG	D	901	1	14,14,15	0.36	0	15,19,21	0.46	0
3	GYK	D	902	-	25,29,29	2.87	7 (28%)	34,42,42	3.61	14 (41%)

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	901	1	-	0/6/23/26	0/1/1/1
3	GYK	A	902	-	-	0/6/32/32	0/3/4/4
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
3	GYK	B	902	-	-	0/6/32/32	0/3/4/4
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
3	GYK	C	902	-	-	0/6/32/32	0/3/4/4
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	GYK	D	902	-	-	0/6/32/32	0/3/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GYK	O26-C25	-5.88	1.32	1.43
3	B	902	GYK	O26-C25	-5.76	1.32	1.43
3	D	902	GYK	O26-C25	-5.74	1.32	1.43
3	C	902	GYK	O26-C25	-5.70	1.32	1.43
3	A	902	GYK	O24-C25	-5.64	1.32	1.43
3	C	902	GYK	O24-C25	-5.59	1.32	1.43
3	D	902	GYK	O24-C25	-5.59	1.32	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	GYK	O24-C25	-5.58	1.32	1.43
3	B	902	GYK	O14-C13	-2.21	1.18	1.23
3	D	902	GYK	O14-C13	-2.20	1.18	1.23
3	C	902	GYK	O14-C13	-2.14	1.18	1.23
3	A	902	GYK	O14-C13	-2.13	1.18	1.23
3	C	902	GYK	C20-N23	2.01	1.45	1.38
3	A	902	GYK	C20-N23	2.02	1.45	1.38
3	A	902	GYK	C05-C04	2.02	1.43	1.39
3	D	902	GYK	C05-C04	2.05	1.43	1.39
3	C	902	GYK	C05-C04	2.13	1.43	1.39
3	C	902	GYK	C17-C10	2.23	1.52	1.49
3	B	902	GYK	C05-C04	2.31	1.43	1.39
3	B	902	GYK	C08-C07	2.44	1.43	1.38
3	A	902	GYK	C08-C07	2.45	1.43	1.38
3	D	902	GYK	C13-N12	2.88	1.45	1.39
3	B	902	GYK	C13-N12	2.99	1.46	1.39
3	C	902	GYK	C13-N12	3.00	1.46	1.39
3	A	902	GYK	C13-N12	3.19	1.46	1.39
3	C	902	GYK	C09-C10	4.42	1.56	1.49
3	B	902	GYK	C09-C10	4.81	1.56	1.49
3	D	902	GYK	C09-C10	4.81	1.56	1.49
3	A	902	GYK	C09-C10	4.85	1.56	1.49
3	D	902	GYK	C13-N15	8.96	1.44	1.34
3	A	902	GYK	C13-N15	9.11	1.45	1.34
3	C	902	GYK	C13-N15	9.32	1.45	1.34
3	B	902	GYK	C13-N15	9.51	1.45	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	902	GYK	C09-C10-N11	-14.02	108.18	126.13
3	D	902	GYK	C09-C10-N11	-13.05	109.42	126.13
3	B	902	GYK	C09-C10-N11	-12.09	110.66	126.13
3	A	902	GYK	C09-C10-N11	-11.34	111.62	126.13
3	D	902	GYK	C09-C10-C17	-7.41	109.19	118.10
3	D	902	GYK	C17-C10-N11	-5.96	107.55	117.79
3	C	902	GYK	C09-C10-C17	-5.42	111.58	118.10
3	C	902	GYK	C17-C10-N11	-4.74	109.65	117.79
3	A	902	GYK	C17-C10-N11	-4.48	110.11	117.79
3	A	902	GYK	O24-C07-C06	-4.45	104.23	109.77
3	B	902	GYK	C17-C10-N11	-4.41	110.22	117.79
3	B	902	GYK	O24-C07-C06	-4.10	104.66	109.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	902	GYK	C16-N15-C13	-3.98	116.78	120.78
3	D	902	GYK	C01-C02-C03	-3.86	107.34	111.43
3	D	902	GYK	O24-C07-C06	-3.71	105.15	109.77
3	C	902	GYK	O24-C07-C06	-3.18	105.81	109.77
3	C	902	GYK	O26-C06-C07	-3.15	105.85	109.77
3	A	902	GYK	C09-C10-C17	-3.06	114.42	118.10
3	B	902	GYK	C01-C02-C03	-2.74	108.54	111.43
3	C	902	GYK	C01-C02-C03	-2.71	108.56	111.43
3	D	902	GYK	O26-C06-C07	-2.64	106.48	109.77
3	A	902	GYK	C01-C02-N12	-2.61	107.91	111.21
3	B	902	GYK	O26-C06-C07	-2.60	106.53	109.77
3	A	902	GYK	C01-C02-C03	-2.47	108.82	111.43
3	A	902	GYK	O26-C06-C07	-2.29	106.91	109.77
3	C	902	GYK	C16-N15-C13	-2.25	118.52	120.78
3	D	902	GYK	O14-C13-N15	-2.24	119.24	123.35
3	A	902	GYK	O14-C13-N15	-2.20	119.33	123.35
3	B	902	GYK	C01-C02-N12	-2.18	108.46	111.21
3	C	902	GYK	C01-C02-N12	-2.02	108.66	111.21
3	A	902	GYK	C05-C04-C09	2.16	122.24	119.29
3	D	902	GYK	C25-O26-C06	2.34	108.74	105.32
3	A	902	GYK	C25-O26-C06	2.40	108.83	105.32
3	B	902	GYK	C25-O26-C06	2.56	109.06	105.32
3	C	902	GYK	C25-O26-C06	2.65	109.18	105.32
3	C	902	GYK	C25-O24-C07	2.73	109.30	105.32
3	D	902	GYK	C25-O24-C07	3.08	109.81	105.32
3	B	902	GYK	C25-O24-C07	3.50	110.44	105.32
3	A	902	GYK	C25-O24-C07	3.74	110.78	105.32
3	A	902	GYK	O26-C06-C05	3.84	133.32	127.87
3	B	902	GYK	O26-C06-C05	4.09	133.67	127.87
3	C	902	GYK	O26-C06-C05	4.13	133.72	127.87
3	D	902	GYK	O26-C06-C05	4.20	133.83	127.87
3	D	902	GYK	C03-C04-C09	4.31	124.65	120.21
3	C	902	GYK	N15-C13-N12	4.32	119.89	115.75
3	C	902	GYK	O24-C07-C08	4.32	133.99	127.87
3	B	902	GYK	N15-C13-N12	4.58	120.15	115.75
3	A	902	GYK	O24-C07-C08	4.73	134.58	127.87
3	B	902	GYK	O24-C07-C08	4.79	134.66	127.87
3	D	902	GYK	O24-C07-C08	4.82	134.70	127.87
3	A	902	GYK	N15-C13-N12	5.71	121.23	115.75
3	D	902	GYK	N15-C13-N12	5.94	121.45	115.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0
3	A	902	GYK	1	0
2	B	901	NAG	1	0
3	B	902	GYK	3	0
2	C	901	NAG	1	0
3	C	902	GYK	3	0
2	D	901	NAG	1	0
3	D	902	GYK	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	773/803 (96%)	-0.12	16 (2%)	67	51	72, 144, 238, 285	0
1	B	773/803 (96%)	-0.13	17 (2%)	65	50	69, 131, 228, 272	0
1	C	773/803 (96%)	0.08	27 (3%)	48	32	101, 167, 232, 261	0
1	D	776/803 (96%)	0.10	36 (4%)	36	24	109, 180, 249, 281	0
All	All	3095/3212 (96%)	-0.02	96 (3%)	52	36	69, 155, 240, 285	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	476	ILE	9.8
1	D	475	ALA	8.0
1	D	544	SER	5.7
1	D	477	ALA	5.7
1	A	782	GLU	5.3
1	D	733	GLY	5.1
1	C	780	SER	4.8
1	A	580	SER	4.7
1	A	400	ILE	4.5
1	D	543	VAL	4.4
1	C	588	GLY	4.3
1	D	779	GLY	4.3
1	B	816	TYR	4.2
1	D	780	SER	4.1
1	B	815	CYS	3.9
1	C	272	GLY	3.9
1	C	784	THR	3.8
1	B	781	LYS	3.8
1	B	588	GLY	3.8
1	B	649	THR	3.7
1	C	684	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	442	LEU	3.5
1	D	175	GLU	3.5
1	B	813	GLU	3.5
1	A	512	PRO	3.4
1	D	453	ARG	3.3
1	D	527	MET	3.3
1	B	104	ASP	3.3
1	A	401	LEU	3.2
1	B	780	SER	3.2
1	C	775	ALA	3.1
1	D	426	VAL	3.0
1	D	384	GLU	3.0
1	C	276	ALA	3.0
1	D	172	LYS	3.0
1	B	456	ASP	3.0
1	A	579	PHE	3.0
1	C	16	GLY	2.9
1	B	775	ALA	2.9
1	D	474	ILE	2.8
1	D	486	GLU	2.8
1	B	144	SER	2.8
1	D	460	TRP	2.8
1	D	732	TYR	2.8
1	A	587	GLN	2.8
1	C	573	ILE	2.7
1	D	485	ARG	2.7
1	D	734	ILE	2.7
1	D	493	LYS	2.7
1	B	476	ILE	2.7
1	A	574	PHE	2.7
1	C	783	LYS	2.7
1	C	410	LYS	2.6
1	C	181	PHE	2.5
1	D	399	THR	2.5
1	A	386	ASP	2.5
1	C	587	GLN	2.5
1	B	587	GLN	2.5
1	D	644	GLU	2.5
1	C	776	LYS	2.4
1	D	441	LYS	2.4
1	C	184	LEU	2.4
1	D	694	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	511	LYS	2.3
1	D	421	TYR	2.3
1	D	408	MET	2.3
1	D	588	GLY	2.3
1	C	577	LEU	2.3
1	D	423	GLY	2.3
1	D	495	PHE	2.3
1	A	543	VAL	2.3
1	D	385	ASP	2.3
1	B	440	TYR	2.3
1	C	17	LEU	2.2
1	C	273	ALA	2.2
1	C	28	ALA	2.2
1	D	587	GLN	2.2
1	B	648	GLY	2.2
1	C	683	VAL	2.2
1	C	265	LEU	2.2
1	C	512	PRO	2.2
1	D	695	LYS	2.2
1	C	341	LEU	2.2
1	D	725	GLY	2.1
1	C	421	TYR	2.1
1	A	523	TYR	2.1
1	A	588	GLY	2.1
1	A	399	THR	2.1
1	C	385	ASP	2.1
1	C	49	ASN	2.1
1	A	781	LYS	2.1
1	A	43	LEU	2.1
1	B	729	SER	2.1
1	D	691	ALA	2.1
1	C	632	PRO	2.0
1	B	11	SER	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, 95^{th} 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	901	14/15	0.62	1.02	6.32	255,255,257,262	0
2	NAG	C	901	14/15	0.27	0.68	5.95	416,416,418,424	0
3	GYK	C	902	26/26	0.75	0.67	4.00	128,169,210,219	0
3	GYK	A	902	26/26	0.81	0.41	0.55	128,169,210,219	0
3	GYK	B	902	26/26	0.91	0.21	-0.29	128,169,210,219	0
3	GYK	D	902	26/26	0.89	0.18	-0.35	128,169,210,219	0
2	NAG	D	901	14/15	0.64	0.38	-	269,269,270,272	0
2	NAG	B	901	14/15	0.70	0.29	-	196,196,199,200	0

6.5 Other polymers (i)

There are no such residues in this entry.