Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:26 PM GMT

PDB ID	:	4IC0
Title	:	Crystal Structure of PAI-1 in Complex with Gallate
Authors	:	Hong, Z.B.; Lin, Z.H.; Gong, L.H.; Huang, M.D.
Deposited on	:	2012-12-09
Resolution	:	2.32 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:

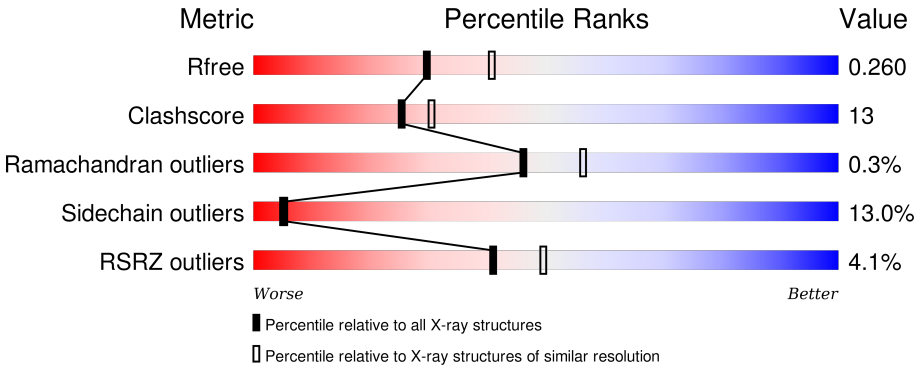
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	379	4% 72% 18% 6%
1	B	379	4% 66% 22% 5% 6%
1	C	379	5% 73% 20%
1	D	379	3% 68% 22% 5%

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	GDE	A	401	-	-	X	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11613 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.

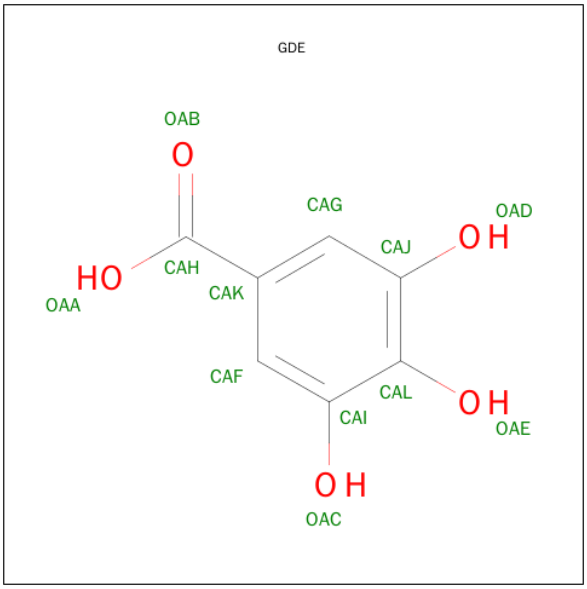
- Molecule 1 is a protein called Plasminogen activator inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2924	1881	499	529	15			
1	B	358	Total	C	N	O	S	0	0	0
			2867	1845	488	520	14			
1	C	366	Total	C	N	O	S	0	0	0
			2924	1881	499	529	15			
1	D	359	Total	C	N	O	S	0	0	0
			2874	1850	489	521	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
A	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
A	158	GLN	ASP	ENGINEERED MUTATION	UNP P05121
A	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
A	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
B	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
B	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
B	158	GLN	ASP	ENGINEERED MUTATION	UNP P05121
B	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
B	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
C	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
C	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
C	158	GLN	ASP	ENGINEERED MUTATION	UNP P05121
C	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
C	354	ILE	MET	ENGINEERED MUTATION	UNP P05121
D	150	HIS	ASN	ENGINEERED MUTATION	UNP P05121
D	154	THR	LYS	ENGINEERED MUTATION	UNP P05121
D	158	GLN	ASP	ENGINEERED MUTATION	UNP P05121
D	319	LEU	GLN	ENGINEERED MUTATION	UNP P05121
D	354	ILE	MET	ENGINEERED MUTATION	UNP P05121

- Molecule 2 is 3,4,5-TRIHYDROXYBENZOIC ACID (three-letter code: GDE) (formula: $C_7H_6O_5$).



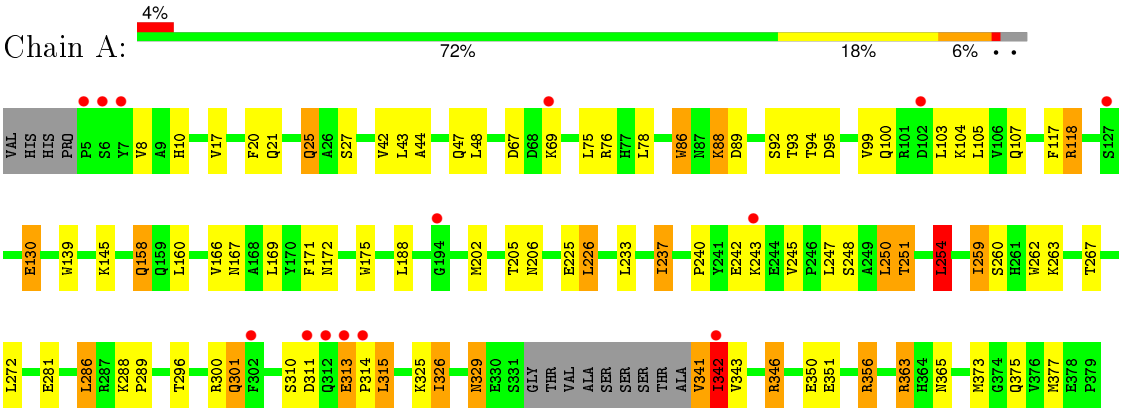
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0

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.

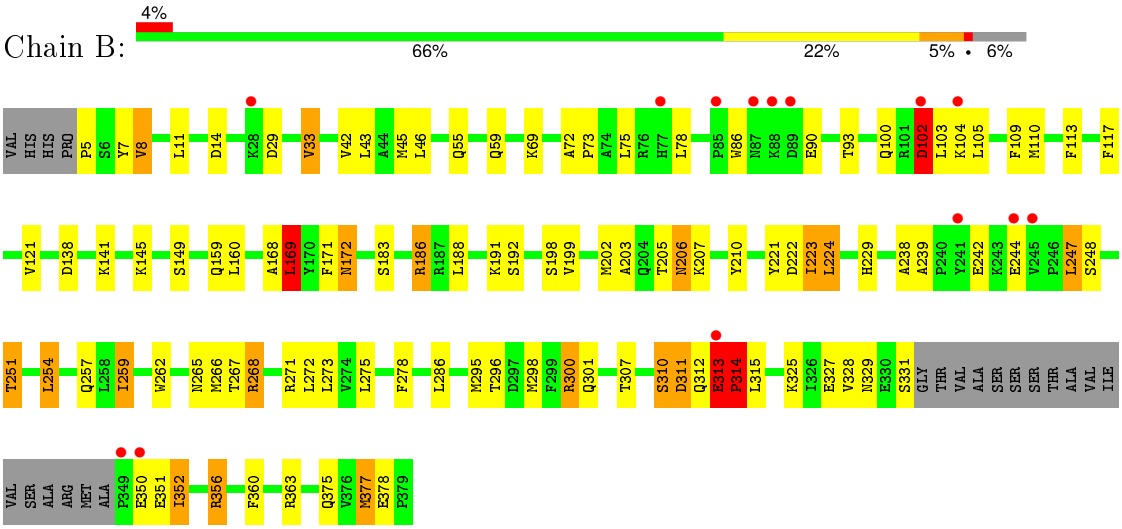
- Molecule 1: Plasminogen activator inhibitor 1

Chain A:



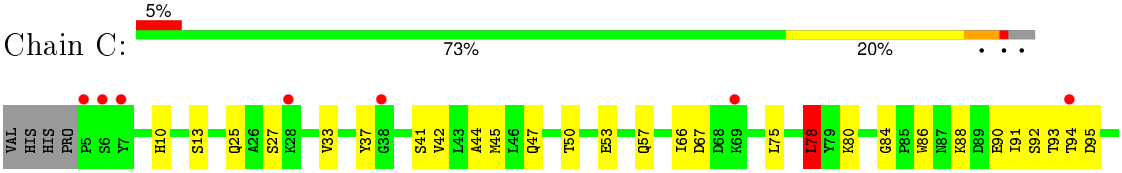
- Molecule 1: Plasminogen activator inhibitor 1

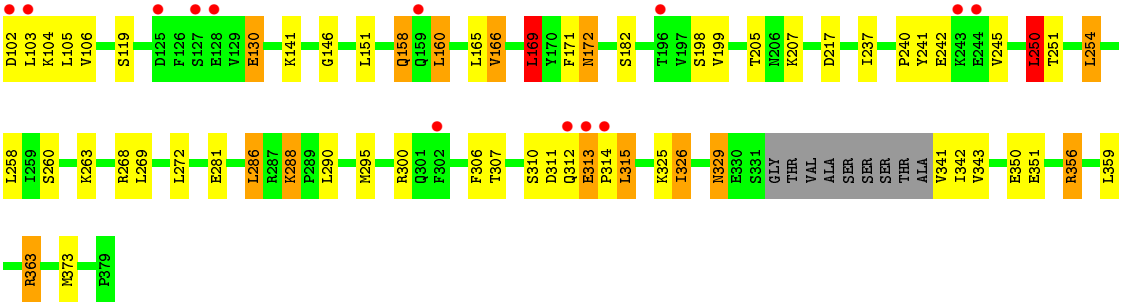
Chain B:



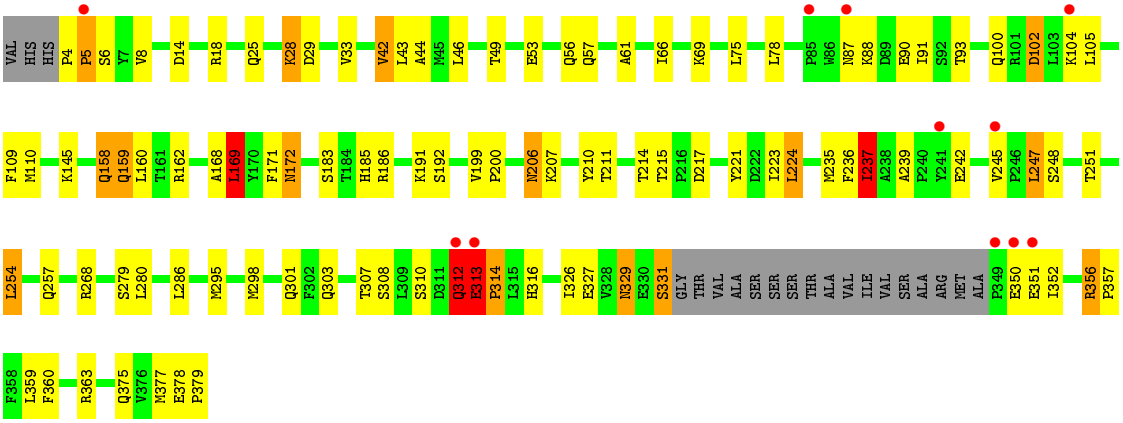
- Molecule 1: Plasminogen activator inhibitor 1

Chain C:





• Molecule 1: Plasminogen activator inhibitor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.28Å 74.99Å 103.87Å 90.91° 93.29° 115.82°	Depositor
Resolution (Å)	38.25 – 2.32 38.25 – 2.32	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.25-2.32) 93.2 (38.25-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.66 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.202 , 0.258 0.210 , 0.260	Depositor DCC
R_{free} test set	3845 reflections (5.59%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 38.1	EDS
Estimated twinning fraction	0.007 for -h,h+k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 72472 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11613	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.375 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: GDE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.04	4/2995 (0.1%)	1.01	10/4060 (0.2%)
1	B	0.99	0/2938	0.95	4/3982 (0.1%)
1	C	1.06	1/2995 (0.0%)	0.98	8/4060 (0.2%)
1	D	0.95	0/2946	0.97	4/3994 (0.1%)
All	All	1.01	5/11874 (0.0%)	0.98	26/16096 (0.2%)

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	1
1	C	0	2
1	D	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	TRP	NE1-CE2	-6.16	1.29	1.37
1	A	139	TRP	CD2-CE2	5.85	1.48	1.41
1	A	175	TRP	CD2-CE2	5.42	1.47	1.41
1	A	262	TRP	CD2-CE2	5.18	1.47	1.41
1	C	86	TRP	CD2-CE2	5.10	1.47	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	169	LEU	CA-CB-CG	8.42	134.67	115.30
1	C	250	LEU	CA-CB-CG	7.71	133.03	115.30
1	C	217	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	343	VAL	CB-CA-C	-7.45	97.24	111.40
1	A	314	PRO	N-CA-C	-6.85	94.29	112.10
1	B	169	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	254	LEU	CA-CB-CG	6.73	130.78	115.30
1	A	343	VAL	N-CA-C	6.64	128.92	111.00
1	B	377	MET	CG-SD-CE	-6.33	90.06	100.20
1	A	342	ILE	CG1-CB-CG2	-6.30	97.54	111.40
1	B	313	GLU	C-N-CD	-6.24	106.88	120.60
1	D	169	LEU	CA-CB-CG	6.05	129.22	115.30
1	C	169	LEU	CB-CG-CD2	5.92	121.07	111.00
1	C	373	MET	CA-CB-CG	5.67	122.95	113.30
1	C	286	LEU	CA-CB-CG	5.67	128.33	115.30
1	D	42	VAL	CB-CA-C	-5.64	100.68	111.40
1	B	314	PRO	CA-N-CD	-5.59	103.67	111.50
1	C	363	ARG	CG-CD-NE	5.59	123.53	111.80
1	C	78	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	342	ILE	C-N-CA	5.41	135.22	121.70
1	A	342	ILE	N-CA-C	5.35	125.45	111.00
1	D	313	GLU	C-N-CD	-5.31	108.92	120.60
1	D	237	ILE	CG1-CB-CG2	-5.29	99.75	111.40
1	A	118	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	202	MET	CG-SD-CE	5.10	108.36	100.20
1	A	286	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	GLU	Peptide
1	A	341	VAL	Peptide
1	B	102	ASP	Peptide
1	C	102	ASP	Peptide
1	C	313	GLU	Peptide
1	D	312	GLN	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	2924	0	2926	83	0
1	B	2867	0	2862	79	0
1	C	2924	0	2926	62	0
1	D	2874	0	2869	69	0
2	A	12	0	2	5	0
2	C	12	0	2	3	0
All	All	11613	0	11587	292	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 13.

All (292) 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:346:ARG:HH11	1:A:346:ARG:CG	1.60	1.14
1:C:158:GLN:HE22	1:C:160:LEU:HB2	1.01	1.07
1:A:205:THR:HG22	1:A:272:LEU:HA	1.33	1.07
1:C:93:THR:HG22	1:C:169:LEU:HD13	1.26	1.06
1:A:93:THR:HG22	1:A:169:LEU:HD23	1.38	1.03
1:D:295:MET:HB3	1:D:298:MET:HE2	1.42	1.01
1:C:93:THR:CG2	1:C:169:LEU:HD13	1.91	0.98
1:B:93:THR:HG22	1:B:169:LEU:CD1	1.94	0.98
1:A:341:VAL:O	1:A:342:ILE:HG13	1.63	0.97
1:B:295:MET:HB3	1:B:298:MET:CE	1.94	0.97
1:C:312:GLN:O	1:C:313:GLU:HG2	1.65	0.97
1:D:206:ASN:HD22	1:D:207:LYS:H	1.13	0.96
1:C:158:GLN:NE2	1:C:160:LEU:HB2	1.82	0.94
1:A:346:ARG:HH11	1:A:346:ARG:HG3	1.31	0.94
1:B:221:TYR:CE1	1:B:223:ILE:HD11	2.04	0.93
1:A:341:VAL:C	1:A:342:ILE:HG13	1.87	0.92
1:D:295:MET:HB3	1:D:298:MET:CE	1.99	0.92
1:B:93:THR:HG22	1:B:169:LEU:HD13	1.53	0.91
1:D:248:SER:HA	1:D:251:THR:OG1	1.69	0.91
1:C:312:GLN:C	1:C:313:GLU:CG	2.39	0.90
1:B:295:MET:HB3	1:B:298:MET:HE2	1.54	0.89
1:C:312:GLN:C	1:C:313:GLU:HG3	1.93	0.89
1:A:346:ARG:HG2	1:A:346:ARG:HH11	1.38	0.88
1:A:346:ARG:HG3	1:A:346:ARG:NH1	1.84	0.87
1:B:5:PRO:HD2	1:B:7:TYR:HB3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:HA	1:A:251:THR:CG2	2.04	0.86
1:A:342:ILE:HD12	1:A:342:ILE:N	1.90	0.86
1:B:206:ASN:HD22	1:B:207:LYS:H	1.24	0.86
1:A:93:THR:CG2	1:A:169:LEU:HD23	2.09	0.83
1:A:341:VAL:O	1:A:342:ILE:CD1	2.29	0.81
1:C:93:THR:HG22	1:C:169:LEU:CD1	2.09	0.81
1:A:341:VAL:O	1:A:342:ILE:CG1	2.29	0.80
1:B:248:SER:HA	1:B:251:THR:OG1	1.81	0.80
1:B:5:PRO:N	1:B:8:VAL:HG22	1.98	0.79
1:A:341:VAL:C	1:A:342:ILE:CG1	2.49	0.79
1:A:42:VAL:HG11	1:A:167:ASN:HB2	1.65	0.78
1:B:93:THR:CG2	1:B:169:LEU:HD13	2.14	0.78
1:B:295:MET:HB3	1:B:298:MET:HE1	1.66	0.78
1:D:104:LYS:H	1:D:312:GLN:NE2	1.81	0.78
1:C:312:GLN:O	1:C:313:GLU:CG	2.30	0.77
1:D:301:GLN:HE21	1:D:316:HIS:CD2	2.00	0.77
1:B:93:THR:HG22	1:B:169:LEU:HD12	1.66	0.77
1:B:29:ASP:OD1	1:B:192:SER:OG	2.01	0.75
1:D:33:VAL:HG12	1:D:360:PHE:HZ	1.50	0.75
1:A:375:GLN:HB2	1:A:377:MET:CE	2.17	0.75
1:D:251:THR:HA	1:D:254:LEU:HD22	1.68	0.74
1:D:191:LYS:NZ	1:D:378:GLU:OE1	2.18	0.74
1:D:295:MET:CB	1:D:298:MET:CE	2.66	0.74
1:B:375:GLN:HB2	1:B:377:MET:HE3	1.68	0.74
1:D:199:VAL:HG11	1:D:379:PRO:HB2	1.69	0.74
1:A:95:ASP:H	2:A:401:GDE:HAF	1.53	0.73
1:A:95:ASP:H	2:A:401:GDE:CAF	2.01	0.73
1:B:251:THR:HA	1:B:254:LEU:CD2	2.19	0.73
1:B:375:GLN:HB2	1:B:377:MET:CE	2.18	0.72
1:B:206:ASN:ND2	1:B:207:LYS:H	1.88	0.72
1:D:162:ARG:NH1	1:D:313:GLU:OE1	2.23	0.71
1:A:342:ILE:N	1:A:342:ILE:CD1	2.47	0.71
1:A:313:GLU:HB2	1:A:315:LEU:HB2	1.71	0.71
1:B:278:PHE:CZ	1:B:328:VAL:HG21	2.25	0.71
1:A:296:THR:HB	1:A:300:ARG:HH21	1.55	0.71
1:B:93:THR:CG2	1:B:169:LEU:CD1	2.68	0.71
1:D:206:ASN:ND2	1:D:207:LYS:H	1.89	0.71
1:C:272:LEU:HD23	1:C:351:GLU:HG2	1.73	0.70
1:D:295:MET:CB	1:D:298:MET:HE2	2.17	0.70
1:A:248:SER:HA	1:A:251:THR:HG22	1.72	0.70
1:D:206:ASN:HD22	1:D:207:LYS:N	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:HG12	1:D:360:PHE:CZ	2.27	0.69
1:A:272:LEU:HD23	1:A:351:GLU:HG2	1.75	0.69
1:B:224:LEU:HD11	1:B:352:ILE:HG21	1.75	0.68
1:A:205:THR:HG22	1:A:272:LEU:CA	2.19	0.68
1:B:221:TYR:HE1	1:B:223:ILE:HD11	1.59	0.68
1:A:313:GLU:O	1:A:313:GLU:HG3	1.91	0.68
1:C:240:PRO:HB3	1:C:245:VAL:HB	1.75	0.68
1:D:313:GLU:N	1:D:314:PRO:HD2	2.07	0.67
1:D:221:TYR:CE1	1:D:223:ILE:HD11	2.30	0.66
1:A:247:LEU:HD12	1:A:377:MET:HE3	1.77	0.66
1:B:141:LYS:HG3	1:B:149:SER:HB3	1.77	0.66
1:C:205:THR:HG22	1:C:272:LEU:HA	1.77	0.65
1:A:247:LEU:HD12	1:A:377:MET:CE	2.25	0.65
1:B:313:GLU:N	1:B:314:PRO:CD	2.58	0.65
1:B:312:GLN:O	1:B:314:PRO:N	2.30	0.65
1:D:375:GLN:HB2	1:D:377:MET:HE3	1.79	0.65
1:B:93:THR:CB	1:B:169:LEU:HD13	2.27	0.64
1:B:295:MET:CB	1:B:298:MET:CE	2.75	0.64
1:C:313:GLU:HB3	1:C:314:PRO:C	2.17	0.64
1:A:346:ARG:CG	1:A:346:ARG:NH1	2.30	0.64
1:A:240:PRO:HB3	1:A:245:VAL:HB	1.80	0.63
1:B:313:GLU:O	1:B:314:PRO:HB2	1.98	0.63
1:A:375:GLN:HB2	1:A:377:MET:HE3	1.78	0.63
1:D:313:GLU:O	1:D:314:PRO:C	2.34	0.63
1:B:5:PRO:HG2	1:B:7:TYR:H	1.65	0.62
1:A:363:ARG:HD2	1:A:365:ASN:OD1	1.98	0.62
1:C:240:PRO:HD2	1:C:356:ARG:HD2	1.82	0.62
1:C:45:MET:CE	1:C:95:ASP:HB3	2.29	0.62
1:D:33:VAL:HG13	1:D:280:LEU:HD12	1.82	0.61
1:A:341:VAL:C	1:A:342:ILE:CD1	2.69	0.61
1:B:312:GLN:C	1:B:314:PRO:N	2.54	0.61
1:C:151:LEU:CD1	1:C:166:VAL:HG21	2.31	0.61
1:D:301:GLN:NE2	1:D:316:HIS:HD2	2.00	0.60
1:C:254:LEU:HD22	1:C:258:LEU:HD23	1.83	0.60
1:A:130:GLU:CD	1:A:130:GLU:H	2.06	0.59
1:B:172:ASN:C	1:B:172:ASN:HD22	2.06	0.59
1:C:151:LEU:HD11	1:C:166:VAL:HG21	1.85	0.59
1:D:329:ASN:HD22	1:D:331:SER:H	1.51	0.59
1:C:95:ASP:CG	2:C:401:GDE:HAF	2.24	0.58
1:B:5:PRO:N	1:B:8:VAL:CG2	2.65	0.58
1:D:301:GLN:NE2	1:D:316:HIS:CD2	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ASP:OD2	2:C:401:GDE:HAF	2.02	0.58
1:D:295:MET:HB3	1:D:298:MET:HE1	1.85	0.58
1:B:206:ASN:HD22	1:B:207:LYS:N	1.99	0.57
1:B:110:MET:HE1	1:B:121:VAL:H	1.69	0.57
1:A:341:VAL:C	1:A:342:ILE:HD12	2.25	0.57
1:D:93:THR:HB	1:D:169:LEU:HD13	1.87	0.57
1:B:45:MET:HE2	1:B:113:PHE:HZ	1.70	0.57
1:A:342:ILE:HD12	1:A:342:ILE:H	1.67	0.56
1:D:221:TYR:CD1	1:D:223:ILE:HD11	2.39	0.56
1:B:5:PRO:CD	1:B:7:TYR:HB3	2.34	0.56
1:C:45:MET:HE1	1:C:95:ASP:CB	2.35	0.56
1:B:100:GLN:HG3	1:B:102:ASP:HB2	1.88	0.56
1:C:130:GLU:H	1:C:130:GLU:CD	2.08	0.56
1:C:313:GLU:HB3	1:C:315:LEU:N	2.20	0.56
1:A:42:VAL:CG1	1:A:167:ASN:HB2	2.36	0.55
1:D:44:ALA:HB1	1:D:66:ILE:HD13	1.87	0.55
1:B:221:TYR:CD1	1:B:223:ILE:HD11	2.42	0.55
1:D:172:ASN:HB2	1:D:327:GLU:HB2	1.88	0.55
1:C:45:MET:CE	1:C:95:ASP:CB	2.84	0.54
1:D:350:GLU:HG2	1:D:351:GLU:H	1.70	0.54
1:B:254:LEU:HD12	1:B:259:ILE:HD11	1.90	0.53
1:A:88:LYS:O	1:A:89:ASP:HB2	2.09	0.53
1:B:313:GLU:O	1:B:314:PRO:CB	2.55	0.53
1:D:307:THR:HA	1:D:310:SER:O	2.09	0.53
1:C:313:GLU:OE1	1:C:315:LEU:HB2	2.09	0.52
1:D:158:GLN:HG2	1:D:159:GLN:N	2.24	0.52
1:A:95:ASP:N	2:A:401:GDE:HAF	2.23	0.52
1:D:295:MET:CB	1:D:298:MET:HE1	2.38	0.52
1:B:247:LEU:HD12	1:B:377:MET:HE3	1.92	0.52
1:B:33:VAL:HG13	1:B:360:PHE:HZ	1.75	0.52
1:B:55:GLN:O	1:B:59:GLN:HG3	2.10	0.51
1:B:295:MET:CB	1:B:298:MET:HE1	2.37	0.51
1:C:45:MET:HE1	1:C:95:ASP:HB3	1.92	0.51
1:C:44:ALA:HB1	1:C:66:ILE:HD13	1.93	0.51
1:C:281:GLU:HB2	1:C:325:LYS:HG2	1.91	0.51
1:A:281:GLU:CB	1:A:325:LYS:HG2	2.40	0.51
1:B:313:GLU:N	1:B:314:PRO:HD2	2.25	0.51
1:A:171:PHE:HD2	1:A:326:ILE:HD12	1.76	0.51
1:A:20:PHE:CD2	1:A:373:MET:CE	2.93	0.51
1:C:207:LYS:HA	1:C:269:LEU:O	2.09	0.51
1:A:247:LEU:O	1:A:251:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLU:O	1:B:171:PHE:HA	2.11	0.51
1:D:104:LYS:H	1:D:312:GLN:HE22	1.55	0.50
1:D:100:GLN:HG3	1:D:102:ASP:HB2	1.93	0.50
1:C:310:SER:O	1:C:313:GLU:OE2	2.29	0.50
1:A:243:LYS:HD3	1:A:356:ARG:NH1	2.25	0.50
1:D:33:VAL:HG11	1:D:326:ILE:CG2	2.42	0.49
1:A:301:GLN:O	1:A:301:GLN:HG2	2.12	0.49
1:B:210:TYR:C	1:B:266:MET:HG2	2.33	0.49
1:D:29:ASP:OD1	1:D:192:SER:OG	2.28	0.49
1:B:307:THR:HA	1:B:310:SER:O	2.12	0.49
1:C:313:GLU:CB	1:C:314:PRO:C	2.80	0.49
1:D:224:LEU:HD11	1:D:352:ILE:HG21	1.95	0.49
1:C:37:TYR:CE1	1:C:78:LEU:HD13	2.47	0.49
1:C:90:GLU:O	1:C:171:PHE:HA	2.12	0.49
1:A:248:SER:HA	1:A:251:THR:HG23	1.92	0.49
1:A:310:SER:O	1:A:313:GLU:OE1	2.29	0.49
1:B:172:ASN:C	1:B:172:ASN:ND2	2.66	0.49
1:C:44:ALA:O	1:C:47:GLN:HB2	2.13	0.49
1:A:243:LYS:HD3	1:A:356:ARG:HH11	1.78	0.49
1:D:236:PHE:O	1:D:360:PHE:HA	2.13	0.49
1:A:329:ASN:C	1:A:329:ASN:HD22	2.16	0.49
1:D:375:GLN:HB2	1:D:377:MET:CE	2.42	0.48
1:D:93:THR:CB	1:D:169:LEU:HD13	2.43	0.48
1:D:33:VAL:CG1	1:D:280:LEU:HD12	2.43	0.48
1:A:92:SER:O	1:A:169:LEU:HA	2.13	0.48
1:C:254:LEU:HD22	1:C:258:LEU:CD2	2.43	0.48
1:B:45:MET:CE	1:B:113:PHE:HZ	2.26	0.48
1:B:202:MET:CE	1:B:275:LEU:HD23	2.44	0.48
1:A:95:ASP:H	2:A:401:GDE:CAI	2.27	0.48
1:A:250:LEU:HD23	1:A:250:LEU:O	2.14	0.48
1:D:53:GLU:O	1:D:57:GLN:HG3	2.14	0.48
1:C:251:THR:CG2	1:C:359:LEU:HD22	2.43	0.48
1:B:109:PHE:CD2	1:B:109:PHE:C	2.87	0.48
1:C:313:GLU:CB	1:C:314:PRO:CA	2.92	0.47
1:A:89:ASP:OD2	1:A:145:LYS:HE2	2.14	0.47
1:A:86:TRP:HH2	1:A:233:LEU:HD11	1.79	0.47
1:B:247:LEU:HD12	1:B:377:MET:CE	2.43	0.47
1:D:357:PRO:HB3	1:D:377:MET:HE1	1.96	0.47
1:C:94:THR:HA	2:C:401:GDE:CAI	2.23	0.47
1:A:99:VAL:HG22	1:A:100:GLN:N	2.29	0.47
1:D:5:PRO:HA	1:D:8:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLU:O	1:C:57:GLN:HG3	2.14	0.47
1:C:151:LEU:CD1	1:C:166:VAL:CG2	2.92	0.47
1:D:4:PRO:O	1:D:8:VAL:HG13	2.15	0.47
1:C:313:GLU:HB3	1:C:315:LEU:HB2	1.96	0.47
1:C:45:MET:HE1	1:C:95:ASP:HB2	1.96	0.47
1:B:242:GLU:HB2	1:B:244:GLU:OE2	2.14	0.47
1:C:182:SER:HB2	1:C:343:VAL:HG22	1.96	0.47
1:A:94:THR:HA	2:A:401:GDE:CAI	2.38	0.47
1:B:272:LEU:HD23	1:B:351:GLU:HG2	1.96	0.47
1:B:311:ASP:N	1:B:311:ASP:OD1	2.47	0.46
1:D:247:LEU:HD12	1:D:377:MET:CE	2.45	0.46
1:D:235:MET:HG2	1:D:237:ILE:HD12	1.96	0.46
1:A:158:GLN:OE1	1:A:160:LEU:HB2	2.15	0.46
1:C:141:LYS:HG3	1:C:146:GLY:HA2	1.97	0.46
1:D:28:LYS:HB2	1:D:28:LYS:HE3	1.48	0.46
1:B:296:THR:O	1:B:300:ARG:HD2	2.16	0.46
1:B:248:SER:HA	1:B:251:THR:HG1	1.79	0.46
1:C:106:VAL:HG22	1:C:311:ASP:OD1	2.16	0.46
1:D:313:GLU:O	1:D:313:GLU:OE2	2.34	0.46
1:C:329:ASN:HD22	1:C:329:ASN:C	2.19	0.46
1:B:46:LEU:HA	1:B:46:LEU:HD12	1.84	0.46
1:D:329:ASN:C	1:D:329:ASN:HD22	2.19	0.45
1:A:226:LEU:HD22	1:A:237:ILE:HD13	1.98	0.45
1:B:186:ARG:HG2	1:B:198:SER:OG	2.16	0.45
1:B:259:ILE:HD12	1:B:262:TRP:CZ3	2.50	0.45
1:A:310:SER:O	1:A:313:GLU:CD	2.55	0.45
1:D:214:THR:HG22	1:D:215:THR:O	2.16	0.45
1:A:247:LEU:CD1	1:A:377:MET:HE1	2.47	0.45
1:D:239:ALA:HB1	1:D:356:ARG:HD2	1.98	0.45
1:B:93:THR:HB	1:B:169:LEU:HD13	1.97	0.45
1:A:225:GLU:C	1:A:226:LEU:HD12	2.37	0.45
1:D:242:GLU:HG3	1:D:245:VAL:HG23	1.99	0.45
1:A:247:LEU:HD12	1:A:377:MET:HE1	1.99	0.44
1:A:20:PHE:CE2	1:A:373:MET:HE2	2.52	0.44
1:A:103:LEU:N	1:A:103:LEU:HD12	2.31	0.44
1:D:46:LEU:HA	1:D:46:LEU:HD12	1.78	0.44
1:B:7:TYR:CZ	1:B:11:LEU:HD11	2.53	0.44
1:D:247:LEU:HD12	1:D:377:MET:HE3	1.99	0.44
1:C:33:VAL:HG11	1:C:326:ILE:CG2	2.48	0.44
1:C:207:LYS:O	1:C:268:ARG:NH1	2.51	0.44
1:C:172:ASN:HD22	1:C:172:ASN:C	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ALA:HB1	1:B:356:ARG:HD2	2.00	0.44
1:A:281:GLU:HB2	1:A:325:LYS:HG2	2.00	0.43
1:A:259:ILE:H	1:A:259:ILE:HG12	1.62	0.43
1:D:295:MET:HB2	1:D:298:MET:CE	2.48	0.43
1:A:20:PHE:CD2	1:A:373:MET:HE1	2.54	0.43
1:B:86:TRP:O	1:B:229:HIS:HE1	2.01	0.43
1:D:49:THR:HG22	1:D:109:PHE:CZ	2.54	0.43
1:A:17:VAL:HG11	1:A:254:LEU:O	2.18	0.43
1:D:199:VAL:HG13	1:D:200:PRO:HD2	2.01	0.43
1:A:226:LEU:CD1	1:A:226:LEU:N	2.82	0.43
1:D:210:TYR:CD2	1:D:211:THR:N	2.86	0.43
1:B:251:THR:HA	1:B:254:LEU:HD23	1.97	0.43
1:D:33:VAL:HG13	1:D:280:LEU:CD1	2.49	0.43
1:D:221:TYR:CD1	1:D:223:ILE:CD1	3.01	0.43
1:B:72:ALA:HB3	1:B:73:PRO:HD3	2.01	0.43
1:D:90:GLU:O	1:D:171:PHE:HA	2.19	0.43
1:A:341:VAL:HG12	1:A:342:ILE:HG23	1.99	0.43
1:D:248:SER:HA	1:D:251:THR:HG1	1.75	0.43
1:C:45:MET:HE2	1:C:95:ASP:CB	2.48	0.43
1:B:45:MET:HA	1:B:117:PHE:CZ	2.54	0.43
1:C:250:LEU:HD13	1:C:359:LEU:HD21	2.00	0.43
1:C:251:THR:HG22	1:C:359:LEU:HD22	2.01	0.43
1:B:350:GLU:HG2	1:B:351:GLU:H	1.84	0.43
1:B:168:ALA:C	1:B:169:LEU:HD22	2.39	0.42
1:B:86:TRP:O	1:B:229:HIS:CE1	2.72	0.42
1:C:104:LYS:HA	1:C:104:LYS:HD3	1.90	0.42
1:C:50:THR:HG22	1:C:306:PHE:CE1	2.55	0.42
1:C:307:THR:HA	1:C:310:SER:O	2.19	0.42
1:D:18:ARG:NH2	1:D:61:ALA:O	2.52	0.42
1:D:168:ALA:C	1:D:169:LEU:HD22	2.39	0.42
1:A:375:GLN:HB2	1:A:377:MET:HE2	1.99	0.42
1:C:45:MET:HE2	1:C:95:ASP:HB3	1.98	0.42
1:C:288:LYS:HD3	1:D:185:HIS:CE1	2.55	0.42
1:A:311:ASP:N	1:A:311:ASP:OD1	2.53	0.42
1:A:205:THR:O	1:A:206:ASN:HB3	2.20	0.42
1:C:313:GLU:HB2	1:C:314:PRO:HA	2.02	0.42
1:C:92:SER:O	1:C:169:LEU:HB3	2.20	0.41
1:A:48:LEU:HD22	1:A:117:PHE:CE1	2.55	0.41
1:C:290:LEU:HD22	1:C:295:MET:CE	2.50	0.41
1:B:205:THR:HA	1:B:271:ARG:O	2.20	0.41
1:C:165:LEU:HD12	1:C:165:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:CD1	1:C:359:LEU:HD21	2.51	0.41
1:B:100:GLN:HE21	1:B:102:ASP:HB2	1.86	0.41
1:A:44:ALA:O	1:A:47:GLN:HB2	2.21	0.41
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.80	0.41
1:A:296:THR:HB	1:A:300:ARG:NH2	2.29	0.41
1:B:45:MET:HE2	1:B:45:MET:HB3	1.88	0.41
1:A:104:LYS:HA	1:A:104:LYS:HE2	2.02	0.41
1:A:288:LYS:HB2	1:A:289:PRO:HD3	2.03	0.41
1:B:191:LYS:HD2	1:B:378:GLU:CD	2.40	0.41
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.79	0.41
1:B:222:ASP:O	1:B:238:ALA:HA	2.20	0.41
1:A:76:ARG:HD3	1:A:118:ARG:HG2	2.03	0.41
1:A:21:GLN:O	1:A:25:GLN:NE2	2.54	0.40
1:A:20:PHE:CD2	1:A:373:MET:HE2	2.56	0.40
1:A:100:GLN:HB3	1:A:103:LEU:HD13	2.03	0.40
1:D:87:ASN:ND2	1:D:91:ILE:HG23	2.37	0.40
1:B:203:ALA:HA	1:B:273:LEU:O	2.22	0.40
1:B:268:ARG:H	1:B:268:ARG:HG3	1.75	0.40
1:B:5:PRO:N	1:B:8:VAL:H	2.20	0.40
1:A:313:GLU:CG	1:A:313:GLU:O	2.66	0.40
1:D:169:LEU:CD2	1:D:169:LEU:N	2.85	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	362/379 (96%)	355 (98%)	7 (2%)	0	100 100
1	B	354/379 (93%)	347 (98%)	5 (1%)	2 (1%)	30 35
1	C	362/379 (96%)	350 (97%)	11 (3%)	1 (0%)	46 56
1	D	355/379 (94%)	348 (98%)	5 (1%)	2 (1%)	30 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1433/1516 (94%)	1400 (98%)	28 (2%)	5 (0%)	46 56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	313	GLU
1	B	314	PRO
1	D	314	PRO
1	D	5	PRO
1	C	84	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	323/333 (97%)	286 (88%)	37 (12%)	7 7
1	B	317/333 (95%)	270 (85%)	47 (15%)	4 3
1	C	323/333 (97%)	282 (87%)	41 (13%)	5 5
1	D	318/333 (96%)	277 (87%)	41 (13%)	5 5
All	All	1281/1332 (96%)	1115 (87%)	166 (13%)	5 5

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	10	HIS
1	A	25	GLN
1	A	27	SER
1	A	43	LEU
1	A	67	ASP
1	A	69	LYS
1	A	75	LEU
1	A	78	LEU
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	107	GLN
1	A	130	GLU
1	A	158	GLN
1	A	166	VAL
1	A	172	ASN
1	A	188	LEU
1	A	226	LEU
1	A	237	ILE
1	A	242	GLU
1	A	250	LEU
1	A	251	THR
1	A	254	LEU
1	A	259	ILE
1	A	260	SER
1	A	263	LYS
1	A	267	THR
1	A	286	LEU
1	A	301	GLN
1	A	315	LEU
1	A	326	ILE
1	A	329	ASN
1	A	342	ILE
1	A	346	ARG
1	A	350	GLU
1	A	356	ARG
1	A	363	ARG
1	B	8	VAL
1	B	14	ASP
1	B	33	VAL
1	B	42	VAL
1	B	43	LEU
1	B	69	LYS
1	B	75	LEU
1	B	78	LEU
1	B	102	ASP
1	B	103	LEU
1	B	104	LYS
1	B	105	LEU
1	B	138	ASP
1	B	145	LYS
1	B	159	GLN

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Mol	Chain	Res	Type
1	B	160	LEU
1	B	169	LEU
1	B	172	ASN
1	B	183	SER
1	B	186	ARG
1	B	199	VAL
1	B	206	ASN
1	B	223	ILE
1	B	224	LEU
1	B	247	LEU
1	B	251	THR
1	B	254	LEU
1	B	257	GLN
1	B	259	ILE
1	B	265	ASN
1	B	267	THR
1	B	268	ARG
1	B	286	LEU
1	B	300	ARG
1	B	301	GLN
1	B	310	SER
1	B	311	ASP
1	B	313	GLU
1	B	314	PRO
1	B	315	LEU
1	B	325	LYS
1	B	327	GLU
1	B	329	ASN
1	B	331	SER
1	B	352	ILE
1	B	356	ARG
1	B	363	ARG
1	C	10	HIS
1	C	13	SER
1	C	25	GLN
1	C	27	SER
1	C	41	SER
1	C	42	VAL
1	C	67	ASP
1	C	75	LEU
1	C	78	LEU
1	C	80	LYS

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Mol	Chain	Res	Type
1	C	88	LYS
1	C	91	ILE
1	C	103	LEU
1	C	105	LEU
1	C	119	SER
1	C	130	GLU
1	C	158	GLN
1	C	160	LEU
1	C	166	VAL
1	C	169	LEU
1	C	172	ASN
1	C	198	SER
1	C	199	VAL
1	C	237	ILE
1	C	241	TYR
1	C	242	GLU
1	C	250	LEU
1	C	254	LEU
1	C	260	SER
1	C	263	LYS
1	C	286	LEU
1	C	288	LYS
1	C	300	ARG
1	C	315	LEU
1	C	326	ILE
1	C	329	ASN
1	C	341	VAL
1	C	342	ILE
1	C	350	GLU
1	C	356	ARG
1	C	363	ARG
1	D	6	SER
1	D	14	ASP
1	D	25	GLN
1	D	28	LYS
1	D	42	VAL
1	D	43	LEU
1	D	56	GLN
1	D	69	LYS
1	D	75	LEU
1	D	78	LEU
1	D	88	LYS

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Mol	Chain	Res	Type
1	D	102	ASP
1	D	105	LEU
1	D	110	MET
1	D	145	LYS
1	D	158	GLN
1	D	159	GLN
1	D	160	LEU
1	D	169	LEU
1	D	172	ASN
1	D	183	SER
1	D	186	ARG
1	D	206	ASN
1	D	217	ASP
1	D	224	LEU
1	D	237	ILE
1	D	247	LEU
1	D	254	LEU
1	D	257	GLN
1	D	268	ARG
1	D	279	SER
1	D	286	LEU
1	D	303	GLN
1	D	308	SER
1	D	312	GLN
1	D	313	GLU
1	D	329	ASN
1	D	331	SER
1	D	356	ARG
1	D	359	LEU
1	D	363	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	172	ASN
1	A	265	ASN
1	A	292	ASN
1	A	301	GLN
1	A	329	ASN
1	A	375	GLN
1	B	172	ASN

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	265	ASN
1	B	292	ASN
1	B	301	GLN
1	B	329	ASN
1	B	375	GLN
1	C	158	GLN
1	C	172	ASN
1	C	265	ASN
1	C	292	ASN
1	C	329	ASN
1	D	159	GLN
1	D	172	ASN
1	D	185	HIS
1	D	206	ASN
1	D	265	ASN
1	D	292	ASN
1	D	312	GLN
1	D	316	HIS
1	D	329	ASN
1	D	375	GLN

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

2 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	GDE	A	401	-	9,12,12	2.95	5 (55%)	12,17,17	2.75	3 (25%)
2	GDE	C	401	-	9,12,12	2.02	3 (33%)	12,17,17	3.69	7 (58%)

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	GDE	A	401	-	-	0/0/4/4	0/1/1/1
2	GDE	C	401	-	-	0/0/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDE	CAI-CAL	-5.26	1.33	1.39
2	A	401	GDE	CAJ-CAL	-5.21	1.33	1.39
2	C	401	GDE	CAJ-CAL	-4.36	1.34	1.39
2	A	401	GDE	OAE-CAL	-2.60	1.30	1.37
2	A	401	GDE	CAG-CAJ	-2.29	1.35	1.38
2	C	401	GDE	CAG-CAK	-2.06	1.36	1.39
2	C	401	GDE	OAC-CAI	2.31	1.41	1.36
2	A	401	GDE	OAC-CAI	2.36	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	GDE	CAF-CAI-CAL	-7.76	115.64	120.42
2	A	401	GDE	CAF-CAI-CAL	-6.37	116.50	120.42
2	C	401	GDE	CAK-CAG-CAJ	-3.91	117.68	120.98
2	C	401	GDE	OAE-CAL-CAJ	-2.69	112.81	119.63
2	A	401	GDE	OAC-CAI-CAF	2.94	127.34	119.42
2	C	401	GDE	CAK-CAF-CAI	3.09	123.59	120.98
2	C	401	GDE	OAC-CAI-CAL	3.13	126.06	117.91
2	C	401	GDE	OAE-CAL-CAI	3.14	127.59	119.63
2	A	401	GDE	CAJ-CAL-CAI	6.09	122.88	119.55
2	C	401	GDE	CAG-CAJ-CAL	7.10	124.81	120.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GDE	5	0
2	C	401	GDE	3	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	366/379 (96%)	0.15	14 (3%)	44	53	17, 30, 54, 85	0
1	B	358/379 (94%)	0.20	14 (3%)	43	52	17, 33, 57, 88	0
1	C	366/379 (96%)	0.23	20 (5%)	29	37	16, 29, 54, 91	0
1	D	359/379 (94%)	0.18	11 (3%)	52	61	16, 33, 55, 94	0
All	All	1449/1516 (95%)	0.19	59 (4%)	41	49	16, 31, 55, 94	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	5.6
1	A	312	GLN	5.6
1	B	313	GLU	4.9
1	C	244	GLU	4.2
1	A	302	PHE	3.9
1	D	313	GLU	3.9
1	C	127	SER	3.9
1	B	241	TYR	3.9
1	A	127	SER	3.8
1	C	6	SER	3.8
1	B	85	PRO	3.6
1	C	7	TYR	3.5
1	C	5	PRO	3.5
1	D	104	LYS	3.3
1	D	5	PRO	3.2
1	A	342	ILE	3.2
1	C	196	THR	3.2
1	A	314	PRO	3.2
1	C	314	PRO	3.0
1	C	69	LYS	2.9
1	B	104	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLU	2.8
1	D	85	PRO	2.7
1	C	302	PHE	2.7
1	D	241	TYR	2.7
1	D	312	GLN	2.7
1	D	350	GLU	2.7
1	C	102	ASP	2.6
1	C	28	LYS	2.6
1	C	103	LEU	2.6
1	D	245	VAL	2.6
1	B	350	GLU	2.5
1	B	244	GLU	2.5
1	C	312	GLN	2.5
1	B	88	LYS	2.5
1	A	6	SER	2.5
1	A	102	ASP	2.4
1	B	245	VAL	2.4
1	A	311	ASP	2.4
1	C	128	GLU	2.3
1	B	102	ASP	2.3
1	D	349	PRO	2.3
1	C	313	GLU	2.3
1	C	125	ASP	2.3
1	D	87	ASN	2.2
1	C	159	GLN	2.2
1	A	69	LYS	2.2
1	A	243	LYS	2.2
1	B	87	ASN	2.1
1	C	38	GLY	2.1
1	B	77	HIS	2.1
1	B	349	PRO	2.1
1	B	89	ASP	2.1
1	A	7	TYR	2.1
1	D	351	GLU	2.1
1	A	194	GLY	2.0
1	B	28	LYS	2.0
1	C	243	LYS	2.0
1	C	94	THR	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	GDE	A	401	12/12	0.68	0.30	4.44	20,20,20,20	0
2	GDE	C	401	12/12	0.76	0.22	1.42	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.