Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:14 PM GMT

PDB ID	:	1EPV
Title	:	ALANINE RACEMASE WITH BOUND INHIBITOR DERIVED FROM D-CYCLOSERINE
Authors	:	Fenn, T.D.; Stamper, G.F.; Morollo, A.A.; Ringe, D.
Deposited on	:	2000-03-29
Resolution	:	2.20 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 (i)) 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 2.20 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.284
Clashscore		12
Ramachandran outliers		0.1%
Sidechain outliers		9.6%
RSRZ outliers		8.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
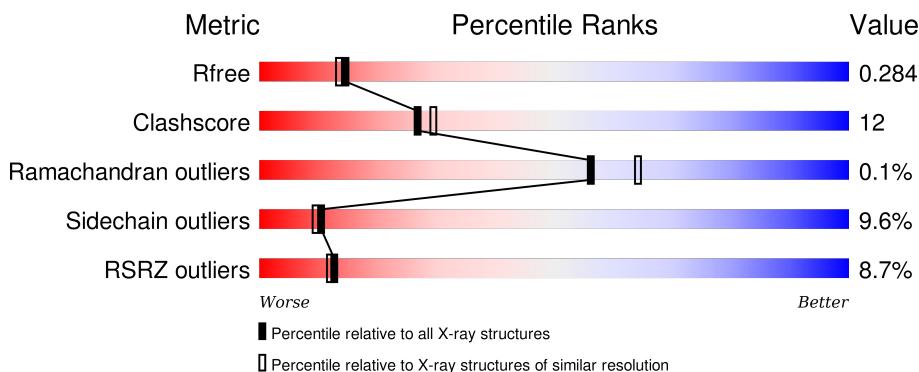
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	387	5% ... 75% ... 20% ...
1	B	387	12% ... 72% ... 19% ... 6%
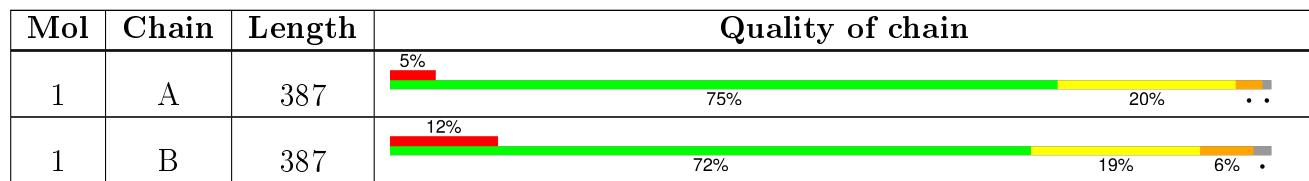
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DCS	A	1001	X	-	X	-
2	DCS	B	1002	X	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6356 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 ALANINE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3033	1941	538	541	13			
1	B	380	Total	C	N	O	S	0	0	0
			3024	1936	536	539	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	KCX	LYS	MODIFIED RESIDUE	UNP P10724
B	129	KCX	LYS	MODIFIED RESIDUE	UNP P10724

- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula: $C_{11}H_{16}N_3O_7P$).
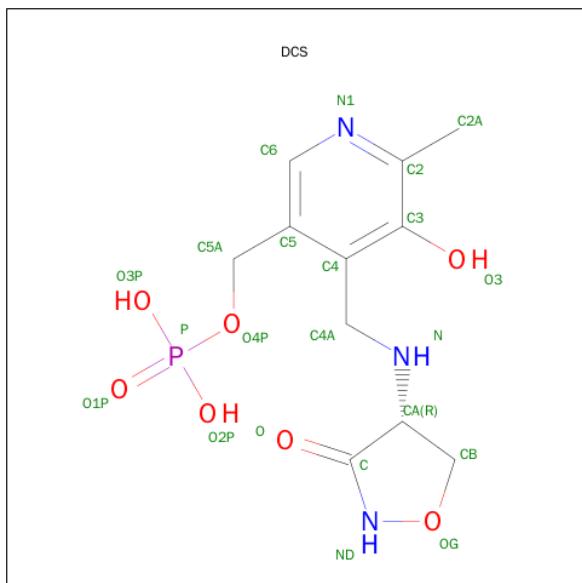
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 11	N 3	O 7	P 1	0	0
2	B	1	Total 22	C 11	N 3	O 7	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total 127	O 127	0	0
3	B	128	Total 128	O 128	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ALANINE RACEMASE
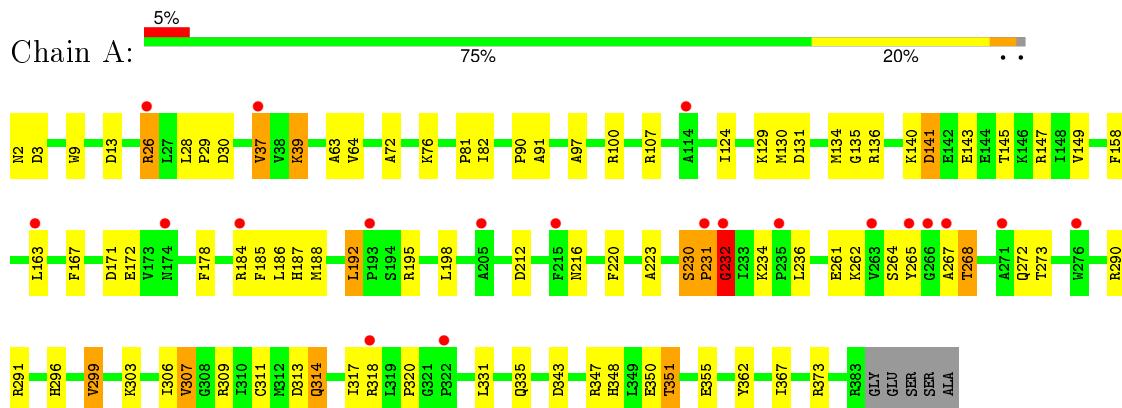
- Molecule 1: ALANINE RACEMASE
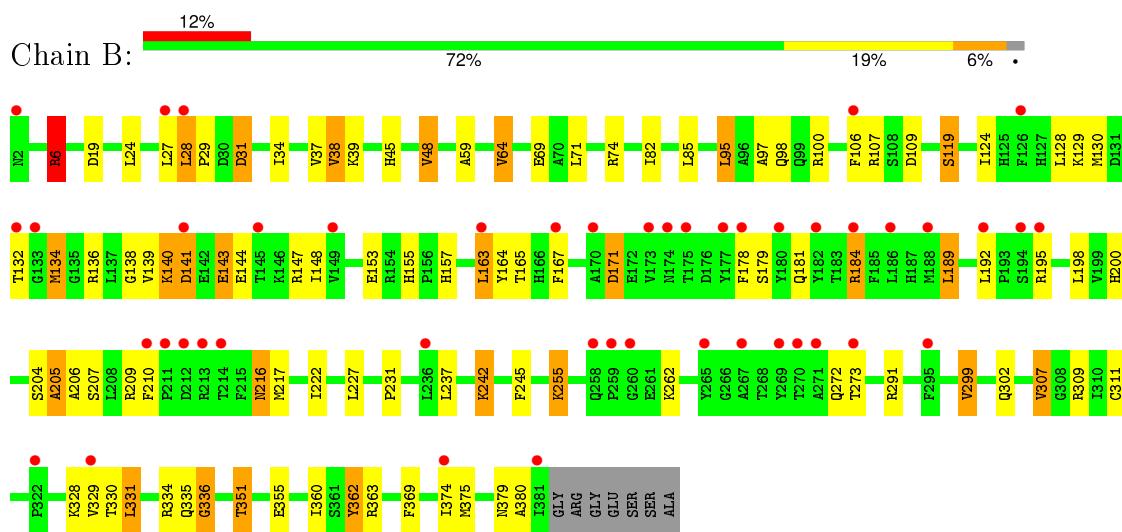
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.16Å 90.24Å 85.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.79 – 2.20 29.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.8 (28.79-2.20) 85.3 (29.58-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.91Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.206 , 0.226 0.287 , 0.284	Depositor DCC
R_{free} test set	1558 reflections (4.33%)	DCC
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 55398 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6356	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.11	11/3098 (0.4%)	1.29	26/4211 (0.6%)
1	B	0.82	1/3089 (0.0%)	1.21	18/4199 (0.4%)
All	All	0.97	12/6187 (0.2%)	1.25	44/8410 (0.5%)

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	2
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	SER	C-N	29.05	1.89	1.34
1	A	231	PRO	C-N	27.49	1.82	1.33
1	B	205	ALA	C-N	14.79	1.68	1.34
1	A	81	PRO	C-N	11.85	1.61	1.34
1	A	30	ASP	C-N	9.67	1.56	1.34
1	A	91	ALA	C-N	8.95	1.54	1.34
1	A	29	PRO	C-N	7.53	1.51	1.34
1	A	82	ILE	C-N	6.99	1.50	1.34
1	A	90	PRO	C-N	6.45	1.48	1.34
1	A	187	HIS	C-N	5.92	1.47	1.34
1	A	186	LEU	C-N	5.79	1.47	1.34
1	A	143	GLU	CG-CD	5.45	1.60	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLY	O-C-N	-16.95	95.58	122.70
1	A	232	GLY	CA-C-N	11.92	143.43	117.20
1	A	30	ASP	O-C-N	-11.61	104.12	122.70
1	A	232	GLY	C-N-CA	10.83	148.78	121.70
1	A	230	SER	C-N-CD	9.79	148.95	128.40
1	A	230	SER	O-C-N	8.46	137.16	121.10
1	A	29	PRO	O-C-N	8.10	135.65	122.70
1	A	82	ILE	O-C-N	7.96	135.43	122.70
1	A	347	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	30	ASP	CA-C-N	7.70	134.14	117.20
1	B	27	LEU	CA-CB-CG	7.50	132.54	115.30
1	A	192	LEU	CA-CB-CG	7.30	132.10	115.30
1	A	347	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	30	ASP	C-N-CA	6.94	139.04	121.70
1	B	307	VAL	N-CA-CB	-6.77	96.60	111.50
1	B	171	ASP	CB-CG-OD1	6.76	124.39	118.30
1	B	98	GLN	CA-CB-CG	6.66	128.06	113.40
1	B	6	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	81	PRO	O-C-N	6.54	133.16	122.70
1	B	209	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	141	ASP	CB-CA-C	-6.31	97.79	110.40
1	B	6	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	109	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	230	SER	CA-C-N	-5.87	100.68	117.10
1	A	29	PRO	CA-C-N	-5.84	104.35	117.20
1	A	82	ILE	CA-C-N	-5.84	104.35	117.20
1	B	209	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	307	VAL	CB-CA-C	5.68	122.20	111.40
1	A	13	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	100	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	363	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	143	GLU	CA-CB-CG	5.39	125.26	113.40
1	A	230	SER	C-N-CA	-5.31	99.72	122.00
1	B	38	VAL	N-CA-CB	-5.28	99.89	111.50
1	A	307	VAL	N-CA-CB	-5.23	99.99	111.50
1	B	307	VAL	CG1-CB-CG2	5.22	119.25	110.90
1	B	360	ILE	N-CA-C	-5.17	97.03	111.00
1	A	29	PRO	C-N-CA	-5.17	108.79	121.70
1	A	81	PRO	CA-C-N	-5.13	105.90	117.20
1	B	184	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	373	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	B	28	LEU	CA-CB-CG	5.02	126.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Mainchain
1	A	362	TYR	Sidechain
1	B	204	SER	Mainchain
1	B	362	TYR	Sidechain

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	3033	0	3015	75	1
1	B	3024	0	3011	79	0
2	A	22	0	12	14	0
2	B	22	0	12	11	0
3	A	127	0	0	10	0
3	B	128	0	0	12	0
All	All	6356	0	6050	143	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 12.

All (143) 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:B:205:ALA:C	1:B:206:ALA:N	1.68	1.46
1:A:231:PRO:C	1:A:232:GLY:N	1.82	1.32
1:A:230:SER:C	1:A:231:PRO:N	1.89	1.25
1:A:147:ARG:NH2	3:A:419:HOH:O	1.64	1.24
1:A:39:LYS:NZ	2:A:1001:DCS:H4A1	1.53	1.22
1:A:163:LEU:CD2	1:A:192:LEU:HD11	1.68	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:NZ	2:B:1002:DCS:H4A1	1.56	1.19
1:A:39:LYS:CE	2:A:1001:DCS:H4A1	1.77	1.13
1:B:141:ASP:OD2	1:B:144:GLU:HB2	1.52	1.07
1:A:163:LEU:HD21	1:A:192:LEU:HD11	1.40	1.03
1:B:39:LYS:HZ1	2:B:1002:DCS:H4A1	0.87	1.01
1:A:39:LYS:HE3	2:A:1001:DCS:H4A1	1.42	1.00
1:A:163:LEU:HD22	1:A:192:LEU:HD11	1.38	0.99
1:A:39:LYS:NZ	2:A:1001:DCS:C4A	2.27	0.98
1:B:39:LYS:HZ1	2:B:1002:DCS:C4A	1.77	0.97
1:B:351:THR:HG21	1:B:355:GLU:OE1	1.67	0.94
1:A:39:LYS:HZ1	2:A:1001:DCS:H4A1	1.14	0.94
1:B:39:LYS:NZ	2:B:1002:DCS:C4A	2.32	0.92
1:A:163:LEU:CD2	1:A:192:LEU:CD1	2.50	0.89
1:A:291:ARG:HH21	1:B:291:ARG:NE	1.69	0.89
1:B:309:ARG:NH1	3:B:653:HOH:O	2.07	0.86
1:A:39:LYS:HZ1	2:A:1001:DCS:C4A	1.85	0.84
1:A:39:LYS:CE	2:A:1001:DCS:C4A	2.57	0.83
1:B:331:LEU:HD23	1:B:331:LEU:N	1.91	0.83
1:A:299:VAL:O	1:A:299:VAL:CG1	2.27	0.83
1:A:2:ASN:N	3:A:440:HOH:O	2.14	0.81
1:A:311:CYS:HB3	2:B:1002:DCS:O	1.81	0.80
1:A:39:LYS:HE3	2:A:1001:DCS:C4A	2.12	0.78
1:A:351:THR:HG21	1:A:355:GLU:OE1	1.83	0.78
1:B:19:ASP:OD2	1:B:242:LYS:HE2	1.84	0.76
1:B:132:THR:O	1:B:181:GLN:HG2	1.87	0.75
1:A:265:TYR:O	3:A:546:HOH:O	2.05	0.74
1:B:328:LYS:NZ	3:B:434:HOH:O	2.21	0.73
1:B:178:PHE:CE2	1:B:210:PHE:CE2	2.75	0.73
1:A:163:LEU:HD21	1:A:192:LEU:CD1	2.15	0.73
1:A:230:SER:C	1:A:231:PRO:CA	2.57	0.72
1:B:141:ASP:OD2	1:B:144:GLU:CB	2.35	0.71
1:A:163:LEU:HD22	1:A:192:LEU:CD1	2.17	0.71
1:B:155:HIS:O	3:B:565:HOH:O	2.07	0.71
1:B:129:KCX:C	1:B:130:MET:CA	2.66	0.70
1:B:299:VAL:HG12	1:B:329:VAL:HG22	1.73	0.70
1:B:334:ARG:NH1	1:B:336:GLY:O	2.25	0.69
1:A:100:ARG:O	3:A:427:HOH:O	2.09	0.69
1:A:350:GLU:HB2	1:B:291:ARG:HH22	1.59	0.68
1:A:299:VAL:O	1:A:299:VAL:HG13	1.94	0.68
1:B:31:ASP:OD2	3:B:447:HOH:O	2.12	0.67
1:A:198:LEU:HA	1:A:216:ASN:HD21	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:HZ3	2:A:1001:DCS:CA	2.08	0.67
1:A:268:THR:HB	3:A:546:HOH:O	1.94	0.67
1:A:291:ARG:NH2	1:B:291:ARG:NE	2.43	0.66
1:B:198:LEU:HA	1:B:216:ASN:HD21	1.60	0.65
1:B:143:GLU:OE2	3:B:633:HOH:O	2.15	0.64
1:A:130:MET:HE3	1:A:185:PHE:CE1	2.33	0.63
1:B:24:LEU:HD23	1:B:34:ILE:HD13	1.81	0.63
1:A:299:VAL:HG12	1:A:299:VAL:O	1.99	0.63
1:A:130:MET:HE3	1:A:185:PHE:CD1	2.34	0.62
1:B:134:MET:HB2	3:B:600:HOH:O	2.00	0.62
1:B:328:LYS:CE	3:B:434:HOH:O	2.49	0.61
1:B:163:LEU:HD13	1:B:192:LEU:HD11	1.82	0.60
1:A:230:SER:CA	1:A:231:PRO:N	2.64	0.60
1:B:129:KCX:CA	1:B:130:MET:N	2.63	0.60
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.66	0.60
1:B:328:LYS:HE3	3:B:434:HOH:O	2.01	0.60
1:B:71:LEU:HD21	1:B:95:LEU:CD1	2.32	0.59
1:B:299:VAL:HG23	1:B:299:VAL:O	2.03	0.59
1:B:167:PHE:CE2	1:B:178:PHE:HE1	2.21	0.59
1:A:130:MET:CE	1:A:185:PHE:CE1	2.87	0.58
1:B:129:KCX:HG2	1:B:138:GLY:HA2	1.86	0.58
1:A:39:LYS:NZ	2:A:1001:DCS:N	2.52	0.58
1:B:143:GLU:CD	3:B:633:HOH:O	2.42	0.58
1:B:39:LYS:HZ3	2:B:1002:DCS:C4A	2.17	0.57
1:A:291:ARG:HH21	1:B:291:ARG:CD	2.18	0.57
1:A:234:LYS:NZ	1:A:343:ASP:OD2	2.37	0.57
1:B:37:VAL:HG12	1:B:39:LYS:HG2	1.88	0.56
1:B:299:VAL:CG1	1:B:329:VAL:HG22	2.34	0.56
1:A:131:ASP:HB3	1:A:140:LYS:HG3	1.87	0.56
1:A:136:ARG:NH1	2:A:1001:DCS:O	2.39	0.55
1:B:85:LEU:HD22	2:B:1002:DCS:H2A3	1.89	0.55
1:A:130:MET:CE	1:A:185:PHE:HE1	2.20	0.54
1:B:129:KCX:OQ1	1:B:136:ARG:NH2	2.25	0.54
1:B:143:GLU:CG	3:B:633:HOH:O	2.55	0.54
1:A:265:TYR:HE2	1:A:311:CYS:HG	1.49	0.54
1:B:132:THR:HG23	1:B:165:THR:OG1	2.08	0.54
1:B:167:PHE:CD2	1:B:178:PHE:HE1	2.27	0.53
1:A:39:LYS:HE3	2:A:1001:DCS:C4	2.38	0.53
1:A:309:ARG:O	3:A:468:HOH:O	2.19	0.53
1:B:134:MET:HB3	3:B:588:HOH:O	2.09	0.53
1:A:220:PHE:CE1	1:A:223:ALA:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HE2	1:B:210:PHE:CE2	2.25	0.52
1:A:130:MET:SD	1:A:188:MET:HB3	2.50	0.52
1:A:311:CYS:HA	2:B:1002:DCS:HND	1.74	0.52
1:A:291:ARG:NH1	1:A:291:ARG:HG3	2.23	0.52
1:A:129:KCX:OQ2	1:A:136:ARG:HB3	2.10	0.51
1:B:119:SER:O	1:B:157:HIS:CE1	2.64	0.51
1:A:171:ASP:OD1	3:A:449:HOH:O	2.19	0.51
1:A:290:ARG:HH11	1:B:351:THR:HG22	1.76	0.51
1:B:74:ARG:CZ	1:B:82:ILE:HD12	2.41	0.51
1:A:291:ARG:HH21	1:B:291:ARG:HE	1.55	0.49
1:B:200:HIS:HB3	1:B:217:MET:HB3	1.95	0.49
1:B:129:KCX:HG2	1:B:138:GLY:CA	2.43	0.49
1:B:178:PHE:CE2	1:B:210:PHE:CD2	3.01	0.49
1:A:37:VAL:HB	1:A:63:ALA:HB3	1.94	0.49
1:B:39:LYS:CE	2:B:1002:DCS:H4A1	2.40	0.48
1:B:39:LYS:NZ	2:B:1002:DCS:N	2.59	0.48
2:A:1001:DCS:O	1:B:311:CYS:HB3	2.14	0.47
1:A:97:ALA:HB2	1:A:124:ILE:HG12	1.96	0.47
1:A:311:CYS:HB3	2:B:1002:DCS:C	2.46	0.46
3:A:517:HOH:O	1:B:262:LYS:HB3	2.13	0.46
1:B:334:ARG:CZ	1:B:336:GLY:O	2.62	0.46
1:B:163:LEU:HD11	1:B:189:LEU:CD1	2.45	0.46
1:A:314:GLN:HG3	1:B:136:ARG:HD2	1.98	0.46
1:A:311:CYS:HB2	1:A:314:GLN:O	2.15	0.46
1:A:296:HIS:CD2	1:A:303:LYS:HD2	2.50	0.46
1:B:330:THR:C	1:B:331:LEU:HD23	2.36	0.45
1:B:45:HIS:NE2	1:B:245:PHE:HB2	2.31	0.45
1:B:34:ILE:HB	1:B:59:ALA:HA	1.99	0.45
1:B:128:LEU:HD13	1:B:148:ILE:HG21	1.99	0.45
1:A:135:GLY:O	1:B:255:LYS:HE2	2.17	0.45
1:B:362:TYR:O	1:B:380:ALA:HB3	2.16	0.45
1:A:320:PRO:HD3	3:A:514:HOH:O	2.15	0.44
1:B:222:ILE:HG13	1:B:227:LEU:HB2	1.99	0.44
1:A:72:ALA:O	1:A:76:LYS:HE2	2.18	0.44
1:A:145:THR:O	1:A:149:VAL:HG23	2.18	0.43
1:A:350:GLU:HB2	1:B:291:ARG:NH2	2.28	0.43
1:A:291:ARG:NH2	1:B:291:ARG:HE	2.11	0.43
1:A:262:LYS:HB3	1:A:267:ALA:HB1	2.02	0.42
1:B:64:VAL:HG13	1:B:69:GLU:HB2	2.01	0.42
1:B:97:ALA:HB2	1:B:124:ILE:HG12	2.01	0.42
1:A:291:ARG:CG	1:A:291:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:TYR:HB2	1:B:200:HIS:O	2.20	0.42
1:A:39:LYS:NZ	2:A:1001:DCS:HB1	2.35	0.42
1:B:334:ARG:HG2	1:B:334:ARG:HH11	1.85	0.42
1:A:124:ILE:HD12	1:A:158:PHE:CE1	2.55	0.42
1:A:306:ILE:HA	1:A:317:ILE:HG22	2.02	0.41
1:A:134:MET:HB3	3:A:482:HOH:O	2.19	0.41
1:A:167:PHE:CD2	1:A:178:PHE:HE1	2.37	0.41
1:A:261:GLU:OE2	1:B:140:LYS:NZ	2.52	0.41
1:B:6:ARG:HD2	3:B:560:HOH:O	2.20	0.41
1:B:29:PRO:HB2	1:B:31:ASP:OD1	2.21	0.41
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.56	0.41
1:B:369:PHE:CE2	1:B:374:ILE:HG12	2.56	0.41
1:B:28:LEU:HA	1:B:29:PRO:HD2	1.91	0.40
1:B:106:PHE:CD2	1:B:107:ARG:HG3	2.56	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:A:26:ARG:NH2	1:A:320:PRO:O[3_546]	1.72	0.48

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	379/387 (98%)	363 (96%)	16 (4%)	0	100	100
1	B	377/387 (97%)	364 (97%)	12 (3%)	1 (0%)	46	50
All	All	756/774 (98%)	727 (96%)	28 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	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	317/321 (99%)	292 (92%)	25 (8%)	15	15
1	B	317/321 (99%)	281 (89%)	36 (11%)	7	6
All	All	634/642 (99%)	573 (90%)	61 (10%)	10	9

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	26	ARG
1	A	37	VAL
1	A	39	LYS
1	A	64	VAL
1	A	107	ARG
1	A	141	ASP
1	A	172	GLU
1	A	184	ARG
1	A	195	ARG
1	A	212	ASP
1	A	236	LEU
1	A	264	SER
1	A	268	THR
1	A	272	GLN
1	A	273	THR
1	A	299	VAL
1	A	307	VAL
1	A	313	ASP
1	A	314	GLN
1	A	318	ARG
1	A	331	LEU
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	348	HIS
1	A	351	THR
1	B	6	ARG
1	B	31	ASP
1	B	38	VAL
1	B	48	VAL
1	B	64	VAL
1	B	95	LEU
1	B	119	SER
1	B	134	MET
1	B	139	VAL
1	B	140	LYS
1	B	141	ASP
1	B	143	GLU
1	B	147	ARG
1	B	153	GLU
1	B	163	LEU
1	B	171	ASP
1	B	179	SER
1	B	184	ARG
1	B	189	LEU
1	B	195	ARG
1	B	207	SER
1	B	216	ASN
1	B	231	PRO
1	B	237	LEU
1	B	242	LYS
1	B	255	LYS
1	B	272	GLN
1	B	273	THR
1	B	299	VAL
1	B	302	GLN
1	B	307	VAL
1	B	331	LEU
1	B	335	GLN
1	B	351	THR
1	B	375	MET
1	B	379	ASN

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

Mol	Chain	Res	Type
1	A	216	ASN
1	A	253	HIS
1	A	272	GLN
1	A	293	GLN
1	A	314	GLN
1	B	216	ASN
1	B	258	GLN
1	B	314	GLN
1	B	379	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	KCX	A	129	1	7,11,12	0.64	0	7,12,14	1.74	1 (14%)
1	KCX	B	129	1	7,11,12	0.80	0	7,12,14	1.29	1 (14%)

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
1	KCX	A	129	1	-	0/6/10/12	0/0/0/0
1	KCX	B	129	1	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	KCX	CE-NZ-CX	-4.28	118.65	123.49
1	B	129	KCX	CE-NZ-CX	2.92	126.81	123.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	KCX	1	0
1	B	129	KCX	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	DCS	A	1001	1	23,23,23	4.71	12 (52%)	24,33,33	1.37	2 (8%)
2	DCS	B	1002	1	23,23,23	4.92	11 (47%)	24,33,33	1.38	1 (4%)

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	DCS	A	1001	1	1/1/3/5	0/10/21/21	0/2/2/2
2	DCS	B	1002	1	1/1/3/5	0/10/21/21	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	DCS	CA-C	-15.47	1.41	1.52
2	A	1001	DCS	CA-C	-13.53	1.42	1.52
2	A	1001	DCS	CB-CA	-6.59	1.37	1.54
2	B	1002	DCS	CB-CA	-6.44	1.37	1.54
2	B	1002	DCS	CA-N	-5.10	1.39	1.47
2	B	1002	DCS	OG-CB	-5.01	1.35	1.44
2	A	1001	DCS	CA-N	-4.89	1.39	1.47
2	A	1001	DCS	OG-CB	-4.78	1.35	1.44
2	B	1002	DCS	OG-ND	-3.48	1.37	1.45
2	A	1001	DCS	OG-ND	-3.09	1.38	1.45
2	B	1002	DCS	C-ND	-2.90	1.30	1.34
2	A	1001	DCS	C4A-C4	-2.79	1.48	1.51
2	A	1001	DCS	C-ND	-2.75	1.31	1.34
2	B	1002	DCS	C5-C4	2.47	1.43	1.40
2	A	1001	DCS	C5-C4	3.09	1.44	1.40
2	B	1002	DCS	O-C	5.47	1.34	1.23
2	B	1002	DCS	P-O3P	6.31	1.77	1.54
2	A	1001	DCS	P-O2P	6.32	1.77	1.54
2	A	1001	DCS	O-C	6.54	1.36	1.23
2	B	1002	DCS	P-O2P	6.62	1.78	1.54
2	A	1001	DCS	P-O3P	6.67	1.78	1.54
2	A	1001	DCS	P-O1P	8.08	1.77	1.51
2	B	1002	DCS	P-O1P	8.65	1.79	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DCS	C4A-C4-C5	-4.15	116.00	119.71
2	A	1001	DCS	C4A-N-CA	3.04	118.46	113.81
2	B	1002	DCS	C4A-N-CA	4.85	121.22	113.81

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1002	DCS	CA
2	A	1001	DCS	CA

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DCS	14	0
2	B	1002	DCS	11	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	381/387 (98%)	0.67	20 (5%)	31	30	10, 22, 42, 57	0
1	B	379/387 (97%)	0.98	46 (12%)	6	5	11, 24, 44, 67	0
All	All	760/774 (98%)	0.82	66 (8%)	13	12	10, 23, 44, 67	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	PRO	5.3
1	B	271	ALA	5.0
1	B	214	THR	4.9
1	B	260	GLY	4.2
1	B	174	ASN	3.9
1	A	26	ARG	3.6
1	A	266	GLY	3.4
1	B	192	LEU	3.3
1	A	263	VAL	3.2
1	B	182	TYR	3.2
1	B	186	LEU	3.1
1	B	267	ALA	3.1
1	B	2	ASN	3.1
1	B	265	TYR	3.1
1	A	322	PRO	3.0
1	B	167	PHE	3.0
1	A	205	ALA	3.0
1	B	184	ARG	3.0
1	B	273	THR	2.9
1	B	374	ILE	2.9
1	A	271	ALA	2.8
1	B	173	VAL	2.7
1	A	235	PRO	2.7
1	A	184	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	276	TRP	2.7
1	B	27	LEU	2.7
1	B	177	TYR	2.7
1	B	213	ARG	2.6
1	B	133	GLY	2.6
1	B	270	THR	2.6
1	B	212	ASP	2.6
1	B	175	THR	2.6
1	B	381	ILE	2.6
1	A	265	TYR	2.5
1	B	258	GLN	2.5
1	B	170	ALA	2.4
1	B	259	PRO	2.3
1	A	174	ASN	2.3
1	A	193	PRO	2.3
1	B	145	THR	2.3
1	B	149	VAL	2.3
1	A	318	ARG	2.3
1	B	195	ARG	2.3
1	B	163	LEU	2.3
1	B	269	TYR	2.3
1	A	114	ALA	2.2
1	A	163	LEU	2.2
1	A	232	GLY	2.2
1	B	180	TYR	2.2
1	B	106	PHE	2.2
1	B	178	PHE	2.2
1	B	236	LEU	2.2
1	A	37	VAL	2.2
1	A	267	ALA	2.2
1	B	126	PHE	2.2
1	B	295	PHE	2.1
1	B	28	LEU	2.1
1	B	141	ASP	2.1
1	B	132	THR	2.1
1	B	322	PRO	2.0
1	B	329	VAL	2.0
1	B	210	PHE	2.0
1	B	211	PRO	2.0
1	A	215	PHE	2.0
1	B	188	MET	2.0
1	B	194	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	KCX	B	129	12/13	0.84	0.22	-	17,24,41,46	0
1	KCX	A	129	12/13	0.84	0.20	-	15,21,26,27	0

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	DCS	B	1002	22/22	0.78	0.26	2.05	14,27,38,46	0
2	DCS	A	1001	22/22	0.86	0.23	0.88	14,20,28,36	0

6.5 Other polymers (i)

There are no such residues in this entry.