Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:44 PM GMT

PDB ID	:	1C8T
Title	:	HUMAN STROMELYSIN-1 (E202Q) CATALYTIC DOMAIN COMPLEXED WITH RO-26-2812
Authors	:	Steele, D.L.; el-Kabbani, O.; Dunten, P.; Crowther, R.L.
Deposited on	:	1999-07-29
Resolution	:	2.60 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:

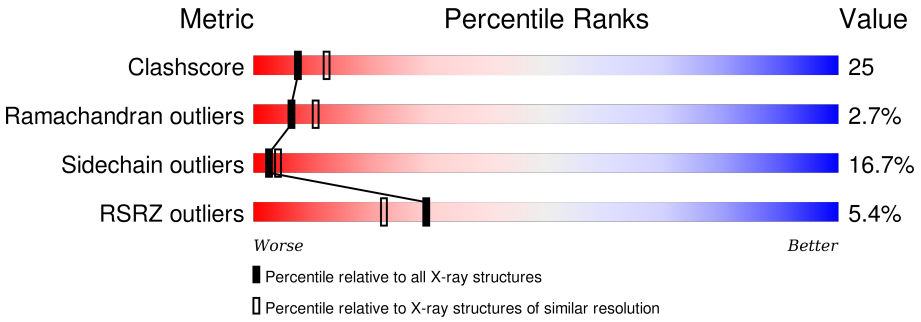
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	167	5% 48% 41% 9% •
1	B	167	5% 44% 47% 7% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2795 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 STROMELYSIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1325	851	220	252	2			
1	B	167	Total	C	N	O	S	0	0	0
			1325	851	220	252	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLN	GLU	ENGINEERED	UNP P08254
B	202	GLN	GLU	ENGINEERED	UNP P08254
A	252	PRO	SER	CONFLICT	UNP P08254
B	252	PRO	SER	CONFLICT	UNP P08254

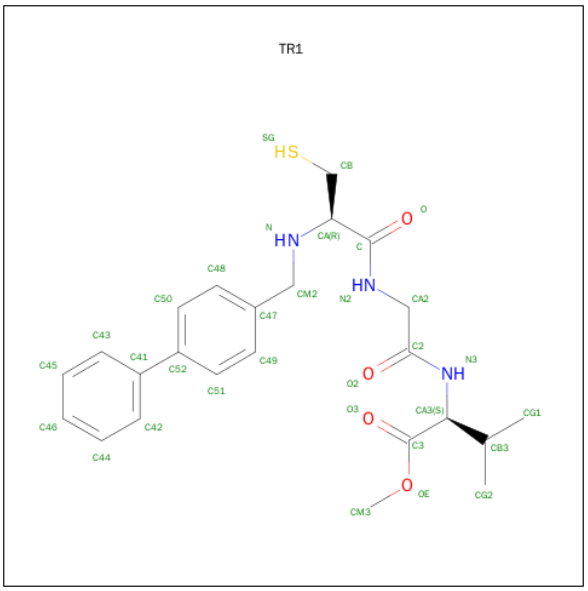
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is 2-(2-{2-[(BIPHENYL-4-YLMETHYL)-AMINO]-3-MERCAPTO-PENTANOYLAMINO}-ACETYLAMINO)-3-METHYL-BUTYRIC ACID METHYL ESTER (three-letter code: TR1) (formula: $C_{24}H_{31}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	24	3	4	1		
4	B	1	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 5 is water.

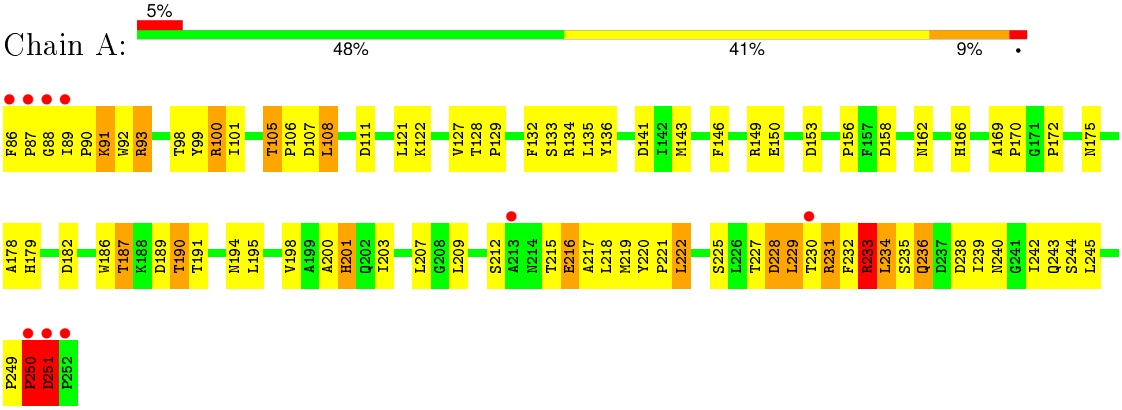
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	35	Total	O	0	0
			35	35		

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.

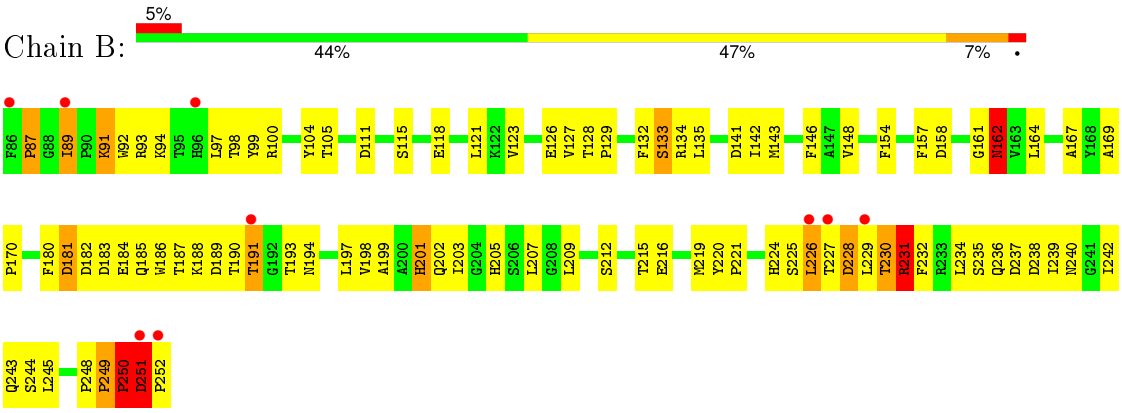
- Molecule 1: STROMELYSIN-1

Chain A:



- Molecule 1: STROMELYSIN-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	120.10Å 47.00Å 54.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 22.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 96.5 (22.05-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.90 (at 2.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , (Not available) 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 9687 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2795	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.86% 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: TR1, ZN, CA

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	0.57	0/1369	1.59	18/1871 (1.0%)
1	B	0.62	0/1369	1.54	10/1871 (0.5%)
All	All	0.60	0/2738	1.57	28/3742 (0.7%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	181	ASP	CB-CG-OD1	14.71	131.54	118.30
1	A	100	ARG	NE-CZ-NH1	-10.63	114.98	120.30
1	A	158	ASP	CB-CG-OD2	9.45	126.80	118.30
1	B	231	ARG	CD-NE-CZ	8.76	135.86	123.60
1	A	153	ASP	CB-CG-OD2	7.25	124.82	118.30
1	B	157	PHE	CB-CG-CD1	-7.23	115.74	120.80
1	A	107	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	A	93	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	A	149	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	231	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	251	ASP	N-CA-CB	-6.51	98.88	110.60
1	B	228	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	A	136	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	141	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	108	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	B	167	ALA	O-C-N	6.00	132.29	122.70
1	A	227	THR	CA-C-O	5.99	132.68	120.10
1	A	143	MET	CA-CB-CG	5.96	123.44	113.30
1	A	136	TYR	CB-CG-CD1	5.89	124.53	121.00
1	A	215	THR	CA-CB-CG2	-5.88	104.17	112.40
1	B	181	ASP	OD1-CG-OD2	-5.85	112.19	123.30
1	A	201	HIS	CA-CB-CG	5.81	123.47	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	HIS	CA-CB-CG	5.78	123.43	113.60
1	A	250	PRO	C-N-CA	5.63	135.78	121.70
1	A	111	ASP	CA-CB-CG	-5.58	101.12	113.40
1	A	233	ARG	CG-CD-NE	5.29	122.91	111.80
1	B	167	ALA	N-CA-CB	5.26	117.46	110.10
1	B	141	ASP	CA-CB-CG	-5.13	102.12	113.40

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	1325	0	1250	65	0
1	B	1325	0	1250	67	0
2	A	2	0	0	0	0
2	B	2	0	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	32	0	30	2	0
4	B	32	0	29	8	0
5	A	36	0	0	4	0
5	B	35	0	0	2	0
All	All	2795	0	2559	133	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 25.

All (133) 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:201:HIS:HA	1:A:218:LEU:HD21	1.49	0.92
2:B:260:ZN:ZN	4:B:265:TR1:HSG	0.63	0.88
1:A:86:PHE:HB2	1:A:87:PRO:HD3	1.59	0.83
1:A:216:GLU:HB3	5:A:18:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LEU:HD11	1:B:242:ILE:HB	1.72	0.70
1:A:231:ARG:HE	1:A:231:ARG:HA	1.55	0.70
1:B:94:LYS:NZ	1:B:97:LEU:HD23	2.05	0.70
4:B:265:TR1:HG13	4:B:265:TR1:C2	2.22	0.69
1:B:249:PRO:O	1:B:251:ASP:N	2.26	0.69
1:A:166:HIS:HB3	1:B:87:PRO:HG2	1.75	0.69
4:B:265:TR1:O2	4:B:265:TR1:HG13	1.93	0.68
1:A:89:ILE:HG12	1:A:91:LYS:HG2	1.76	0.68
1:A:150:GLU:HA	1:A:156:PRO:HB3	1.75	0.66
1:B:209:LEU:HB2	1:B:219:MET:HE2	1.79	0.65
1:A:201:HIS:CA	1:A:218:LEU:HD21	2.24	0.65
1:B:236:GLN:HA	1:B:239:ILE:HD12	1.79	0.63
1:A:218:LEU:HD23	1:A:219:MET:SD	2.38	0.63
1:B:198:VAL:HA	4:B:265:TR1:H48	1.80	0.63
1:A:201:HIS:HA	1:A:218:LEU:CD2	2.26	0.62
1:A:231:ARG:NE	1:A:231:ARG:HA	2.11	0.62
1:B:228:ASP:OD1	1:B:231:ARG:HD2	1.99	0.62
1:B:94:LYS:HZ2	1:B:97:LEU:HD23	1.62	0.62
1:A:169:ALA:HB1	1:A:170:PRO:HD2	1.81	0.62
1:A:232:PHE:O	1:A:233:ARG:NE	2.35	0.58
1:A:239:ILE:O	1:A:243:GLN:HG3	2.03	0.58
1:B:238:ASP:O	1:B:242:ILE:HG22	2.04	0.58
1:B:134:ARG:HD2	5:B:71:HOH:O	2.02	0.58
1:A:134:ARG:HG3	1:A:135:LEU:N	2.19	0.57
1:A:187:THR:O	1:A:194:ASN:HA	2.04	0.57
1:B:248:PRO:C	1:B:250:PRO:HD2	2.25	0.57
1:B:251:ASP:N	1:B:252:PRO:HD3	2.19	0.57
1:B:199:ALA:O	1:B:203:ILE:HG12	2.04	0.57
1:B:100:ARG:HB3	1:B:143:MET:SD	2.44	0.56
1:A:221:PRO:HG2	1:A:222:LEU:HD22	1.88	0.56
1:A:172:PRO:O	1:A:175:ASN:HB2	2.04	0.56
1:A:249:PRO:HB2	1:A:251:ASP:CB	2.36	0.56
1:A:128:THR:HB	1:A:129:PRO:CD	2.35	0.56
1:A:190:THR:HB	1:A:225:SER:HB3	1.86	0.56
1:B:194:ASN:OD1	1:B:197:LEU:HG	2.06	0.55
1:B:209:LEU:HD11	1:B:242:ILE:HD13	1.88	0.55
1:B:226:LEU:HD12	1:B:231:ARG:O	2.06	0.55
1:A:234:LEU:HD13	1:A:238:ASP:HB2	1.89	0.55
1:A:249:PRO:HB2	1:A:251:ASP:HB2	1.88	0.54
1:A:87:PRO:HG3	4:B:265:TR1:SG	2.48	0.54
1:B:186:TRP:HZ3	1:B:198:VAL:HG21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:THR:HG22	5:A:15:HOH:O	2.07	0.54
1:A:228:ASP:O	1:A:230:THR:N	2.41	0.54
1:B:129:PRO:HG3	1:B:252:PRO:HD2	1.89	0.54
1:A:100:ARG:HG2	1:A:101:ILE:N	2.24	0.53
1:B:235:SER:C	1:B:237:ASP:H	2.12	0.53
1:A:98:THR:HB	1:A:135:LEU:HD13	1.90	0.52
1:A:249:PRO:O	1:A:250:PRO:C	2.48	0.52
1:A:128:THR:CB	1:A:129:PRO:CD	2.87	0.52
1:B:99:TYR:HA	1:B:142:ILE:O	2.10	0.51
1:B:92:TRP:CE2	1:B:170:PRO:HB3	2.45	0.51
1:B:164:LEU:HD21	4:B:265:TR1:HM33	1.93	0.51
1:B:187:THR:HG21	1:B:191:THR:HB	1.92	0.51
1:B:104:TYR:HB3	5:B:21:HOH:O	2.10	0.51
1:B:134:ARG:HG3	1:B:135:LEU:N	2.26	0.51
1:B:194:ASN:HB3	1:B:197:LEU:HD12	1.92	0.51
1:B:158:ASP:OD2	1:B:162:ASN:HB3	2.11	0.51
1:B:189:ASP:CG	1:B:190:THR:H	2.14	0.51
1:A:221:PRO:HG2	1:A:222:LEU:CD2	2.41	0.50
1:A:233:ARG:HA	1:A:233:ARG:CZ	2.41	0.50
1:B:118:GLU:HA	1:B:121:LEU:HD12	1.93	0.50
1:A:217:ALA:HB1	1:A:238:ASP:OD2	2.12	0.50
1:B:181:ASP:OD1	1:B:183:ASP:HB2	2.12	0.49
1:B:127:VAL:C	1:B:128:THR:HG23	2.32	0.49
1:B:249:PRO:N	1:B:250:PRO:HD2	2.28	0.49
1:B:169:ALA:HB1	1:B:170:PRO:HD2	1.93	0.49
1:B:98:THR:HA	1:B:133:SER:O	2.12	0.49
1:A:238:ASP:O	1:A:242:ILE:HG22	2.13	0.49
1:A:234:LEU:HB3	1:A:239:ILE:HG13	1.95	0.48
1:A:98:THR:HB	1:A:135:LEU:CD1	2.43	0.48
1:A:99:TYR:CZ	1:A:134:ARG:HB2	2.49	0.48
1:A:150:GLU:CA	1:A:156:PRO:HB3	2.44	0.48
1:A:189:ASP:OD1	1:A:191:THR:OG1	2.27	0.48
1:B:97:LEU:O	1:B:132:PHE:HA	2.14	0.48
1:A:222:LEU:N	1:A:222:LEU:HD22	2.28	0.48
1:B:105:THR:HB	1:B:146:PHE:CE1	2.48	0.48
1:A:162:ASN:HA	5:A:65:HOH:O	2.13	0.48
1:A:121:LEU:HD22	1:A:132:PHE:CD1	2.48	0.48
1:B:235:SER:C	1:B:237:ASP:N	2.67	0.47
1:A:129:PRO:HA	1:A:250:PRO:HD2	1.97	0.47
4:B:265:TR1:CG1	4:B:265:TR1:C2	2.93	0.47
5:A:14:HOH:O	1:B:87:PRO:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:CD1	1:A:170:PRO:HB3	2.50	0.46
1:A:236:GLN:NE2	1:A:240:ASN:OD1	2.49	0.46
1:B:220:TYR:CD2	1:B:221:PRO:HD2	2.51	0.46
1:B:129:PRO:HB3	1:B:251:ASP:HA	1.98	0.46
1:B:94:LYS:HZ1	1:B:97:LEU:HD23	1.79	0.46
1:A:128:THR:HB	1:A:129:PRO:HD2	1.99	0.45
1:A:203:ILE:O	1:A:207:LEU:HG	2.15	0.45
1:A:209:LEU:HD21	1:A:242:ILE:HA	1.98	0.45
1:A:229:LEU:C	1:A:231:ARG:N	2.70	0.45
1:B:89:ILE:HD12	1:B:91:LYS:HG2	1.99	0.45
1:A:229:LEU:C	1:A:231:ARG:H	2.19	0.44
1:A:132:PHE:CD2	1:A:132:PHE:N	2.86	0.44
1:B:209:LEU:HD11	1:B:242:ILE:CD1	2.48	0.44
1:B:161:GLY:O	1:B:162:ASN:C	2.56	0.43
1:B:129:PRO:CB	1:B:251:ASP:HA	2.48	0.43
1:A:146:PHE:HZ	1:A:195:LEU:HD21	1.84	0.43
1:A:217:ALA:HA	1:A:235:SER:OG	2.18	0.43
1:B:105:THR:HB	1:B:146:PHE:CD1	2.53	0.43
1:A:236:GLN:HA	1:A:239:ILE:HB	2.00	0.43
1:B:123:VAL:O	1:B:234:LEU:HD11	2.19	0.43
1:B:243:GLN:C	1:B:245:LEU:N	2.72	0.43
1:A:219:MET:O	1:A:220:TYR:C	2.57	0.42
1:A:191:THR:H	1:A:191:THR:HG1	1.61	0.42
1:B:98:THR:HG21	1:B:135:LEU:HD21	2.01	0.42
1:B:180:PHE:N	1:B:180:PHE:CD2	2.88	0.42
1:B:92:TRP:HB3	1:B:94:LYS:HG2	2.02	0.42
1:B:134:ARG:O	1:B:135:LEU:HD23	2.19	0.42
1:A:93:ARG:NH1	1:B:154:PHE:O	2.47	0.42
1:A:200:ALA:CB	1:A:218:LEU:HD11	2.50	0.42
1:B:226:LEU:C	1:B:228:ASP:N	2.72	0.42
1:A:108:LEU:HD21	1:A:187:THR:HA	2.02	0.42
1:A:108:LEU:HG	1:A:186:TRP:O	2.20	0.41
1:B:205:HIS:O	1:B:207:LEU:N	2.53	0.41
1:B:201:HIS:NE2	4:B:265:TR1:N	2.69	0.41
1:B:234:LEU:O	1:B:235:SER:C	2.59	0.41
1:B:123:VAL:O	1:B:127:VAL:HG22	2.20	0.41
1:A:105:THR:HA	1:A:106:PRO:HD3	1.88	0.41
1:A:217:ALA:O	4:A:265:TR1:H45	2.19	0.41
1:B:89:ILE:HG13	1:B:89:ILE:H	1.51	0.41
1:B:198:VAL:O	1:B:202:GLN:HG2	2.20	0.41
1:B:230:THR:O	1:B:232:PHE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:HIS:CB	1:B:87:PRO:HG2	2.47	0.40
1:B:240:ASN:O	1:B:243:GLN:N	2.53	0.40
1:A:178:ALA:O	1:A:179:HIS:HD2	2.04	0.40
1:A:198:VAL:HA	4:A:265:TR1:H48	2.03	0.40
1:B:181:ASP:HB3	1:B:184:GLU:HG2	2.03	0.40
1:B:243:GLN:O	1:B:245:LEU:N	2.54	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	165/167 (99%)	148 (90%)	13 (8%)	4 (2%)	7 13
1	B	165/167 (99%)	139 (84%)	21 (13%)	5 (3%)	5 8
All	All	330/334 (99%)	287 (87%)	34 (10%)	9 (3%)	6 10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	B	250	PRO
1	B	251	ASP
1	B	227	THR
1	A	88	GLY
1	A	250	PRO
1	B	162	ASN
1	A	251	ASP
1	B	87	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	141/141 (100%)	121 (86%)	20 (14%)	4 7
1	B	141/141 (100%)	114 (81%)	27 (19%)	2 3
All	All	282/282 (100%)	235 (83%)	47 (17%)	3 4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	91	LYS
1	A	105	THR
1	A	122	LYS
1	A	127	VAL
1	A	133	SER
1	A	182	ASP
1	A	187	THR
1	A	190	THR
1	A	212	SER
1	A	216	GLU
1	A	222	LEU
1	A	228	ASP
1	A	231	ARG
1	A	233	ARG
1	A	234	LEU
1	A	236	GLN
1	A	244	SER
1	A	245	LEU
1	A	251	ASP
1	B	89	ILE
1	B	91	LYS
1	B	93	ARG
1	B	111	ASP
1	B	115	SER
1	B	126	GLU
1	B	133	SER

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Mol	Chain	Res	Type
1	B	148	VAL
1	B	162	ASN
1	B	182	ASP
1	B	185	GLN
1	B	188	LYS
1	B	191	THR
1	B	193	THR
1	B	212	SER
1	B	215	THR
1	B	216	GLU
1	B	224	HIS
1	B	225	SER
1	B	226	LEU
1	B	229	LEU
1	B	230	THR
1	B	231	ARG
1	B	244	SER
1	B	249	PRO
1	B	250	PRO
1	B	251	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	236	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TR1	A	265	2	33,33,33	1.11	3 (9%)	42,43,43	2.31	12 (28%)
4	TR1	B	265	2	33,33,33	1.19	4 (12%)	42,43,43	3.06	19 (45%)

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
4	TR1	A	265	2	-	0/34/34/34	0/2/2/2
4	TR1	B	265	2	-	0/34/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	265	TR1	C52-C41	-3.31	1.40	1.49
4	B	265	TR1	C52-C41	-3.01	1.41	1.49
4	B	265	TR1	CA3-N3	-2.93	1.39	1.45
4	B	265	TR1	C-N2	2.09	1.38	1.33
4	A	265	TR1	C2-N3	2.16	1.38	1.34
4	B	265	TR1	CA-N	2.32	1.50	1.47
4	A	265	TR1	CA-N	2.73	1.51	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	265	TR1	CA-CB-SG	-6.20	106.53	114.16
4	A	265	TR1	OE-C3-O3	-4.98	113.50	123.79
4	A	265	TR1	CM2-N-CA	-4.37	107.13	113.81
4	B	265	TR1	OE-C3-O3	-4.01	115.51	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	265	TR1	CA2-N2-C	-3.92	112.42	121.26
4	A	265	TR1	O-C-CA	-3.56	112.50	120.36
4	B	265	TR1	CB3-CA3-N3	-3.54	102.03	111.36
4	A	265	TR1	CA3-N3-C2	-3.15	115.58	121.78
4	B	265	TR1	CM2-N-CA	-2.96	109.28	113.81
4	B	265	TR1	CA-CB-SG	-2.77	110.75	114.16
4	B	265	TR1	CA2-C2-N3	-2.66	109.42	116.12
4	B	265	TR1	C50-C48-C47	-2.45	117.69	121.04
4	A	265	TR1	CB3-CA3-N3	-2.42	104.96	111.36
4	A	265	TR1	C51-C49-C47	-2.40	117.75	121.04
4	B	265	TR1	C47-CM2-N	-2.38	106.61	112.69
4	B	265	TR1	C49-C51-C52	-2.15	118.00	121.14
4	A	265	TR1	O2-C2-N3	-2.14	119.38	123.01
4	B	265	TR1	O-C-N2	-2.13	118.80	123.08
4	B	265	TR1	O3-C3-CA3	-2.02	117.81	124.30
4	B	265	TR1	O2-C2-CA2	2.34	125.42	120.66
4	A	265	TR1	OE-C3-CA3	2.91	123.08	111.95
4	A	265	TR1	CB3-CA3-C3	2.95	120.08	111.63
4	B	265	TR1	CG2-CB3-CA3	3.34	121.14	111.14
4	B	265	TR1	C2-CA2-N2	3.78	123.75	113.26
4	B	265	TR1	OE-C3-CA3	3.83	126.61	111.95
4	B	265	TR1	CB-CA-C	4.06	118.81	109.66
4	B	265	TR1	CB-CA-N	4.67	117.95	111.40
4	A	265	TR1	O-C-N2	4.68	132.48	123.08
4	B	265	TR1	C3-CA3-N3	6.09	126.34	109.52
4	A	265	TR1	CA2-N2-C	6.48	135.89	121.26
4	B	265	TR1	CA3-N3-C2	12.81	146.99	121.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	265	TR1	2	0
4	B	265	TR1	8	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	167/167 (100%)	0.13	9 (5%) 29 22	4, 15, 33, 54	0
1	B	167/167 (100%)	0.12	9 (5%) 29 22	4, 13, 29, 39	0
All	All	334/334 (100%)	0.12	18 (5%) 29 22	4, 14, 30, 54	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	PRO	8.5
1	B	251	ASP	6.6
1	A	252	PRO	6.5
1	A	251	ASP	4.8
1	B	191	THR	4.0
1	A	86	PHE	3.9
1	A	230	THR	3.8
1	B	227	THR	3.8
1	A	88	GLY	3.2
1	A	250	PRO	3.2
1	B	86	PHE	3.1
1	A	87	PRO	2.9
1	A	89	ILE	2.9
1	B	226	LEU	2.6
1	A	213	ALA	2.5
1	B	89	ILE	2.4
1	B	96	HIS	2.3
1	B	229	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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
4	TR1	A	265	32/32	0.86	0.22	0.67	7,21,32,34	0
4	TR1	B	265	32/32	0.89	0.21	0.06	11,20,28,29	0
3	CA	A	264	1/1	0.96	0.14	-0.52	12,12,12,12	0
3	CA	B	264	1/1	0.97	0.12	-0.58	20,20,20,20	0
3	CA	B	262	1/1	0.95	0.10	-1.10	14,14,14,14	0
2	ZN	B	260	1/1	0.97	0.07	-1.55	21,21,21,21	0
3	CA	B	263	1/1	0.97	0.11	-1.87	15,15,15,15	0
3	CA	A	263	1/1	0.96	0.08	-2.11	13,13,13,13	0
3	CA	A	262	1/1	0.91	0.08	-2.21	13,13,13,13	0
2	ZN	A	261	1/1	0.99	0.07	-5.13	14,14,14,14	0
2	ZN	B	261	1/1	1.00	0.07	-6.75	10,10,10,10	0
2	ZN	A	260	1/1	0.98	0.07	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.