



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:51 AM GMT

PDB ID : 3N95
Title : Crystal structure of human CRFR2 alpha extracellular domain in complex with Urocortin 2
Authors : Pal, K.; Swaminathan, K.; Pioszak, A.A.; Xu, H.E.
Deposited on : 2010-05-28
Resolution : 2.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

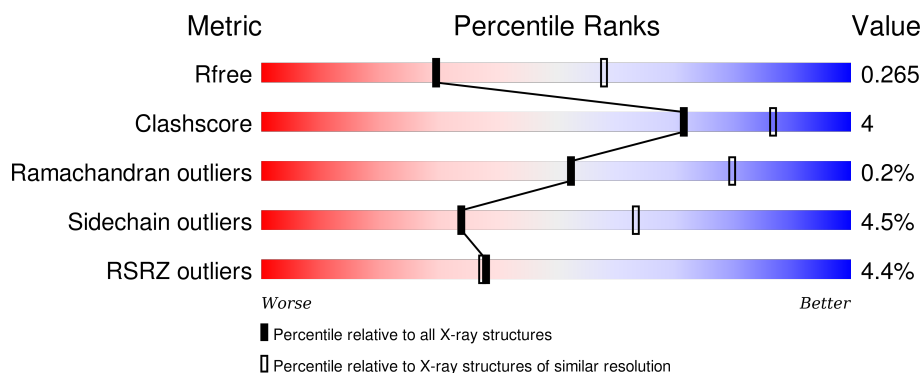
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	<div> <div>0%</div> <div>86% 11% .</div> </div>
1	B	482	<div> <div>2%</div> <div>85% 12% ..</div> </div>
1	C	482	<div> <div>2%</div> <div>84% 11% . .</div> </div>
1	D	482	<div> <div>11%</div> <div>84% 11% .</div> </div>
2	E	17	<div> <div>18%</div> <div>94% 6%</div> </div>

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Mol	Chain	Length	Quality of chain	
			6%	12%
2	F	17	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '6%', a green segment in the middle labeled '88%', and a yellow segment at the end labeled '12%'. The total length of the bar represents 100%.	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15086 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 Maltose binding protein-CRFR2 alpha extracellular domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3643	2335	594	702	12			
1	B	472	Total	C	N	O	S	0	0	0
			3659	2347	596	704	12			
1	C	462	Total	C	N	O	S	0	0	0
			3584	2297	585	690	12			
1	D	463	Total	C	N	O	S	0	0	0
			3592	2301	586	693	12			

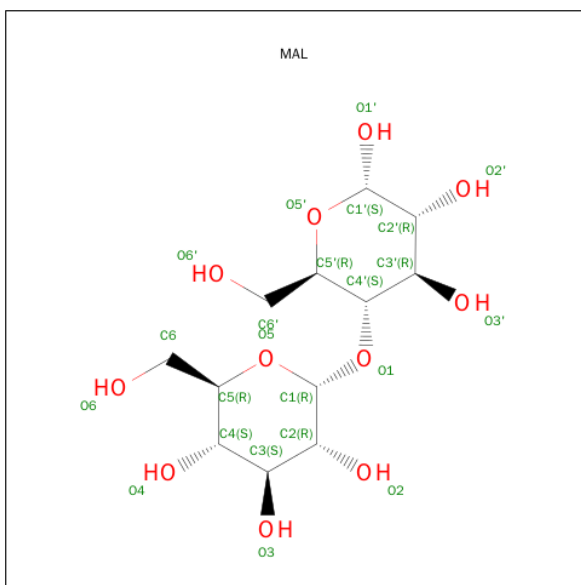
- Molecule 2 is a protein called Urocortin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	0	0	1
			122	72	28	22			
2	F	17	Total	C	N	O	0	0	1
			122	72	28	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	42	NH2	-	AMIDATION	UNP Q96RP3
F	42	NH2	-	AMIDATION	UNP Q96RP3

- Molecule 3 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		
3	C	1	Total	C	O	0	0
			23	12	11		
3	D	1	Total	C	O	0	0
			23	12	11		

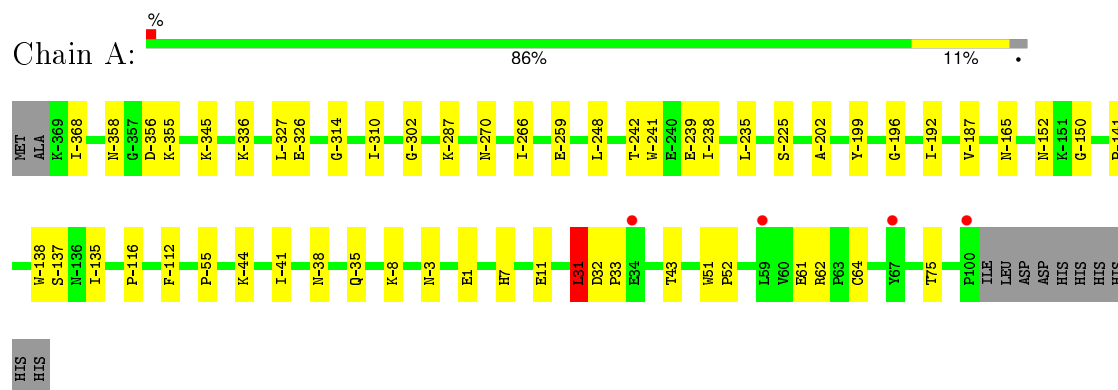
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	B	65	Total	O	0	0
			65	65		
4	C	61	Total	O	0	0
			61	61		
4	D	47	Total	O	0	0
			47	47		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		

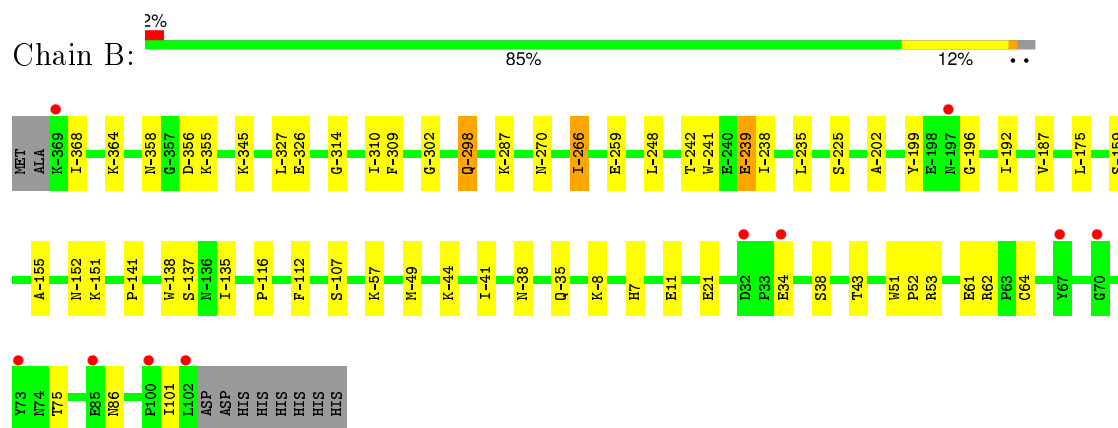
3 Residue-property plots

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.

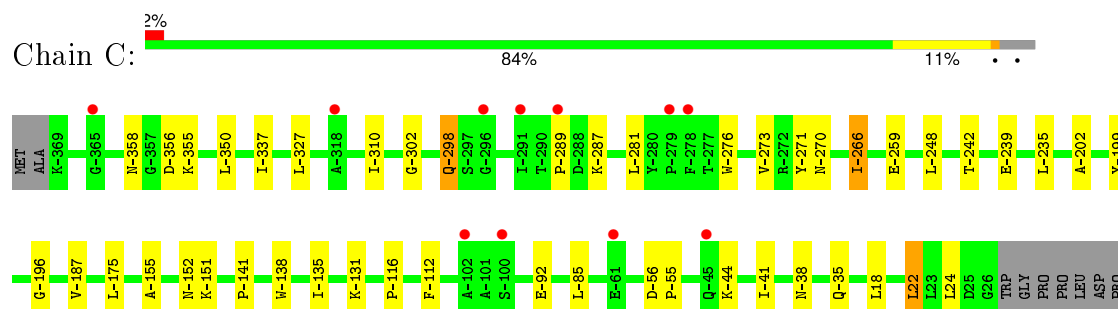
- Molecule 1: Maltose binding protein-CRFR2 alpha extracellular domain



- Molecule 1: Maltose binding protein-CRFR2 alpha extracellular domain



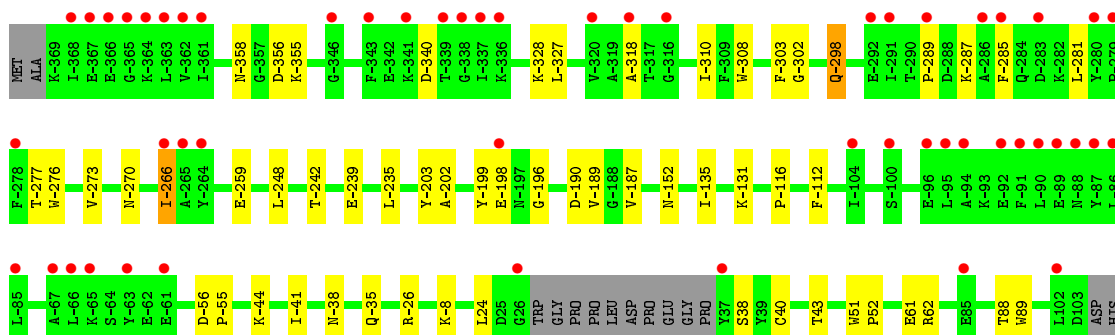
- Molecule 1: Maltose binding protein-CRFR2 alpha extracellular domain





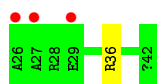
- Molecule 1: Maltose binding protein-CRFR2 alpha extracellular domain

Chain D: 11% 84% 11%



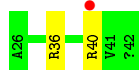
- Molecule 2: Urocortin-2

Chain E: 18% 94% 6%



- Molecule 2: Urocortin-2

Chain F: 6% 88% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.31Å 212.07Å 107.32Å 90.00° 104.54° 90.00°	Depositor
Resolution (Å)	50.00 – 2.72 47.22 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.72) 98.4 (47.22-2.72)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.224 , 0.266 0.223 , 0.265	Depositor DCC
R_{free} test set	3151 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 9.6	EDS
Estimated twinning fraction	0.358 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62074 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15086	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAL, NH2

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	0.55	0/3735	0.59	1/5082 (0.0%)
1	B	0.54	0/3751	0.60	0/5104
1	C	0.53	1/3669 (0.0%)	0.61	3/4986 (0.1%)
1	D	0.51	0/3677	0.59	0/4997
2	E	0.40	0/120	0.53	0/161
2	F	0.44	0/120	0.56	0/161
All	All	0.53	1/15072 (0.0%)	0.60	4/20491 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	-92	GLU	CB-CG	-6.32	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-92	GLU	N-CA-CB	-5.56	100.59	110.60
1	C	-92	GLU	CA-CB-CG	5.56	125.63	113.40
1	C	38	SER	N-CA-C	5.27	125.24	111.00
1	A	31	LEU	CA-CB-CG	5.26	127.40	115.30

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	3643	0	3559	27	1
1	B	3659	0	3581	29	0
1	C	3584	0	3515	39	0
1	D	3592	0	3519	38	1
2	E	122	0	128	0	0
2	F	122	0	128	4	0
3	A	23	0	22	0	0
3	B	23	0	22	0	0
3	C	23	0	22	0	0
3	D	23	0	22	0	0
4	A	97	0	0	5	0
4	B	65	0	0	1	0
4	C	61	0	0	11	0
4	D	47	0	0	13	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	15086	0	14518	126	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 4.

All (126) 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)
4:A:608:HOH:O	1:C:37:TYR:HB3	1.39	1.21
1:D:-318:ALA:HB1	2:F:36:ARG:HD2	1.47	0.95
1:A:-192:ILE:HD12	1:C:38:SER:HB3	1.54	0.87
1:A:-165:ASN:HB2	4:A:215:HOH:O	1.75	0.86
1:D:-38:ASN:HB2	4:D:314:HOH:O	1.77	0.83
1:C:-298:GLN:HE21	1:C:-298:GLN:HA	1.44	0.83
1:B:-192:ILE:HD12	1:D:38:SER:HB3	1.63	0.80
1:C:-350:LEU:HA	4:C:640:HOH:O	1.81	0.79
1:D:-318:ALA:CB	2:F:36:ARG:HD2	2.12	0.79
1:D:-203:TYR:CE1	4:D:532:HOH:O	2.36	0.77
1:C:37:TYR:O	1:C:37:TYR:CD2	2.39	0.76
1:A:-302:GLY:HA3	1:A:-38:ASN:O	1.91	0.70
1:D:-298:GLN:HE21	1:D:-298:GLN:HA	1.56	0.70
1:D:-199:TYR:OH	1:D:-196:GLY:HA2	1.92	0.69
1:B:-302:GLY:HA3	1:B:-38:ASN:O	1.93	0.68
1:C:101:ILE:HG23	4:C:202:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:O	4:C:536:HOH:O	2.11	0.67
1:C:-298:GLN:CA	1:C:-298:GLN:HE21	2.08	0.66
1:B:86:ASN:HB2	1:D:-198:GLU:CD	2.16	0.66
1:C:-302:GLY:HA3	1:C:-38:ASN:O	1.97	0.65
1:C:-38:ASN:HB2	4:C:425:HOH:O	1.96	0.65
1:D:-277:THR:OG1	4:D:729:HOH:O	2.13	0.65
1:D:-285:PHE:HD1	4:D:535:HOH:O	1.80	0.64
1:D:-302:GLY:HA3	1:D:-38:ASN:O	1.98	0.64
1:A:-242:THR:OG1	1:A:-239:GLU:HG2	1.99	0.62
1:D:-242:THR:OG1	1:D:-239:GLU:HG3	1.99	0.62
1:C:-152:ASN:HD21	1:C:-135:ILE:HG12	1.65	0.62
1:C:-199:TYR:OH	1:C:-196:GLY:HA2	2.00	0.61
1:D:-203:TYR:CD1	4:D:532:HOH:O	2.53	0.60
1:B:86:ASN:HB2	1:D:-198:GLU:OE2	2.01	0.59
1:D:-152:ASN:HD21	1:D:-135:ILE:HG12	1.67	0.59
1:D:-190:ASP:O	4:D:532:HOH:O	2.17	0.58
1:B:-199:TYR:OH	1:B:-196:GLY:HA2	2.04	0.58
1:D:52:PRO:HD3	1:D:62:ARG:HD3	1.86	0.57
1:D:-281:LEU:HD12	1:D:-276:TRP:CZ2	2.38	0.57
1:B:-242:THR:OG1	1:B:-239:GLU:HG2	2.05	0.57
1:C:37:TYR:HA	4:C:536:HOH:O	2.03	0.56
1:C:91:SER:HB3	4:C:406:HOH:O	2.05	0.56
1:A:51:TRP:CZ3	1:A:62:ARG:HG2	2.40	0.56
1:A:-199:TYR:OH	1:A:-196:GLY:HA2	2.07	0.55
1:A:52:PRO:HD3	1:A:62:ARG:HD3	1.88	0.54
1:A:-3:ASN:O	1:A:1:GLU:HG3	2.07	0.54
1:B:51:TRP:CZ3	1:B:62:ARG:HG2	2.43	0.54
1:A:-368:ILE:HG12	1:A:-314:GLY:O	2.08	0.54
1:D:51:TRP:CZ3	1:D:62:ARG:HG2	2.44	0.53
1:B:52:PRO:HD3	1:B:62:ARG:HD3	1.90	0.53
1:B:-152:ASN:HD21	1:B:-135:ILE:HG12	1.73	0.53
1:C:51:TRP:CZ3	1:C:62:ARG:HG2	2.44	0.52
1:B:86:ASN:HB2	1:D:-198:GLU:OE1	2.09	0.52
1:C:-289:PRO:O	4:C:438:HOH:O	2.19	0.52
2:F:36:ARG:HB3	2:F:40:ARG:HH12	1.75	0.52
1:A:31:LEU:O	1:A:33:PRO:HD3	2.10	0.52
1:C:-298:GLN:NE2	1:C:-298:GLN:HA	2.21	0.51
1:C:-248:LEU:HD21	1:C:-235:LEU:HD11	1.92	0.51
1:C:-242:THR:OG1	1:C:-239:GLU:HG3	2.11	0.51
1:A:-150:GLY:HA2	4:A:130:HOH:O	2.10	0.51
1:A:7:HIS:NE2	1:A:11:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-248:LEU:HD21	1:B:-235:LEU:HD11	1.93	0.50
1:C:-350:LEU:HD12	4:C:640:HOH:O	2.10	0.50
1:A:-336:LYS:HE2	4:A:282:HOH:O	2.10	0.50
1:D:-358:ASN:ND2	1:D:-356:ASP:OD1	2.45	0.50
1:D:-318:ALA:HB1	2:F:36:ARG:CD	2.33	0.49
1:B:-155:ALA:O	1:B:-151:LYS:HB2	2.12	0.49
1:A:-192:ILE:HD12	1:C:38:SER:CB	2.34	0.49
1:D:-302:GLY:N	4:D:314:HOH:O	2.46	0.49
1:A:-326:GLU:N	1:A:-326:GLU:OE1	2.44	0.48
1:C:86:ASN:ND2	4:C:113:HOH:O	2.46	0.48
1:A:-248:LEU:HD21	1:A:-235:LEU:HD11	1.96	0.48
1:D:-302:GLY:CA	4:D:314:HOH:O	2.62	0.48
1:B:-355:LYS:HE3	1:B:-259:GLU:OE2	2.14	0.48
1:B:38:SER:HA	4:B:305:HOH:O	2.14	0.48
1:A:-152:ASN:HD21	1:A:-135:ILE:HG12	1.79	0.47
1:B:-57:LYS:NZ	1:C:-337:ILE:HD11	2.29	0.47
1:C:52:PRO:HD3	1:C:62:ARG:HD3	1.97	0.47
1:B:-298:GLN:OE1	1:D:88:THR:HG21	2.14	0.47
1:A:32:ASP:HB2	4:A:117:HOH:O	2.14	0.47
1:B:-326:GLU:N	1:B:-326:GLU:OE1	2.45	0.47
1:B:7:HIS:NE2	1:B:11:GLU:OE1	2.49	0.46
1:C:-358:ASN:ND2	1:C:-356:ASP:OD1	2.49	0.46
1:D:-248:LEU:HD21	1:D:-235:LEU:HD11	1.97	0.46
1:C:-116:PRO:HB3	1:C:-44:LYS:HD3	1.98	0.46
1:B:-298:GLN:HA	1:B:-298:GLN:NE2	2.31	0.46
1:D:-289:PRO:HB2	4:D:535:HOH:O	2.16	0.45
1:C:-355:LYS:HE3	1:C:-259:GLU:OE2	2.16	0.45
1:D:40:CYS:HB3	1:D:89:TRP:CE2	2.51	0.45
1:D:-308:TRP:HB3	1:D:-303:PHE:HE1	1.81	0.45
1:C:-155:ALA:O	1:C:-151:LYS:HB2	2.17	0.45
1:D:-56:ASP:HA	1:D:-55:PRO:HD2	1.88	0.45
1:C:-298:GLN:CA	1:C:-298:GLN:NE2	2.78	0.45
1:D:-26:ARG:CZ	4:D:394:HOH:O	2.64	0.45
1:A:-355:LYS:HE3	1:A:-259:GLU:OE2	2.17	0.45
1:B:21:GLU:HG3	1:B:53:ARG:HB2	1.98	0.45
1:C:-281:LEU:HD12	1:C:-276:TRP:CZ2	2.51	0.45
1:A:-241:TRP:HA	1:A:-238:ILE:HD12	1.98	0.44
1:D:-203:TYR:HE1	4:D:532:HOH:O	1.86	0.44
1:C:62:ARG:NH2	4:C:452:HOH:O	2.51	0.44
1:D:-328:LYS:HE2	4:D:385:HOH:O	2.16	0.44
1:D:-273:VAL:O	1:D:-266:ILE:HG13	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-358:ASN:ND2	1:B:-356:ASP:OD1	2.48	0.43
1:A:-141:PRO:HA	1:A:-138:TRP:CE2	2.53	0.43
1:C:-298:GLN:HG2	1:C:-271:TYR:OH	2.19	0.43
1:B:-368:ILE:HG12	1:B:-314:GLY:O	2.19	0.43
1:D:-116:PRO:HB3	1:D:-44:LYS:HD3	2.01	0.43
1:A:-116:PRO:HB3	1:A:-44:LYS:HD3	2.00	0.43
1:B:-116:PRO:HB3	1:B:-44:LYS:HD3	2.00	0.43
1:A:61:GLU:O	1:A:62:ARG:HD2	2.20	0.42
1:C:-273:VAL:O	1:C:-266:ILE:HG13	2.20	0.42
1:C:-56:ASP:HA	1:C:-55:PRO:HD2	1.92	0.42
1:B:64:CYS:O	1:B:75:THR:HG22	2.20	0.42
1:B:-241:TRP:HA	1:B:-238:ILE:HD12	2.00	0.42
1:C:37:TYR:C	4:C:536:HOH:O	2.55	0.42
1:D:-189:VAL:HA	4:D:532:HOH:O	2.19	0.41
1:A:64:CYS:O	1:A:75:THR:HG22	2.20	0.41
1:D:-298:GLN:NE2	1:D:-298:GLN:HA	2.32	0.41
1:A:-358:ASN:ND2	1:A:-356:ASP:OD1	2.50	0.41
1:B:-309:PHE:HA	1:B:-107:SER:O	2.20	0.41
1:C:-141:PRO:HA	1:C:-138:TRP:CE2	2.55	0.41
1:A:51:TRP:CE3	1:A:62:ARG:HG2	2.56	0.41
1:C:-266:ILE:H	1:C:-266:ILE:HG13	1.78	0.41
1:B:-141:PRO:HA	1:B:-138:TRP:CE2	2.56	0.41
1:D:-355:LYS:HE3	1:D:-259:GLU:OE2	2.21	0.41
1:C:37:TYR:HD2	1:C:37:TYR:O	1.97	0.40
1:B:-49:MET:CE	1:B:-49:MET:HA	2.51	0.40
1:B:-266:ILE:HG13	1:B:-266:ILE:H	1.77	0.40
1:A:-266:ILE:HG13	1:A:-266:ILE:H	1.74	0.40
1:C:18:LEU:HG	1:C:22:LEU:HD22	2.03	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:-55:PRO:CD	1:D:-340:ASP:O[1_455]	2.12	0.08

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	468/482 (97%)	460 (98%)	7 (2%)	1 (0%)	52	80
1	B	470/482 (98%)	461 (98%)	8 (2%)	1 (0%)	52	80
1	C	458/482 (95%)	449 (98%)	8 (2%)	1 (0%)	52	80
1	D	459/482 (95%)	448 (98%)	10 (2%)	1 (0%)	52	80
2	E	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
2	F	15/17 (88%)	15 (100%)	0	0	100	100
All	All	1885/1962 (96%)	1847 (98%)	34 (2%)	4 (0%)	52	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-202	ALA
1	A	-202	ALA
1	D	-202	ALA
1	B	-202	ALA

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	377/388 (97%)	363 (96%)	14 (4%)	41	71
1	B	379/388 (98%)	357 (94%)	22 (6%)	25	51
1	C	371/388 (96%)	354 (95%)	17 (5%)	33	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	372/388 (96%)	357 (96%)	15 (4%)	38	68
2	E	11/11 (100%)	10 (91%)	1 (9%)	12	26
2	F	11/11 (100%)	11 (100%)	0	100	100
All	All	1521/1574 (97%)	1452 (96%)	69 (4%)	34	63

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-345	LYS
1	A	-327	LEU
1	A	-310	ILE
1	A	-287	LYS
1	A	-270	ASN
1	A	-225	SER
1	A	-187	VAL
1	A	-137	SER
1	A	-112	PHE
1	A	-41	ILE
1	A	-35	GLN
1	A	-8	LYS
1	A	31	LEU
1	A	43	THR
1	B	-364	LYS
1	B	-345	LYS
1	B	-327	LEU
1	B	-310	ILE
1	B	-298	GLN
1	B	-287	LYS
1	B	-270	ASN
1	B	-266	ILE
1	B	-239	GLU
1	B	-225	SER
1	B	-187	VAL
1	B	-175	LEU
1	B	-159	SER
1	B	-137	SER
1	B	-112	PHE
1	B	-41	ILE
1	B	-35	GLN
1	B	-8	LYS
1	B	34	GLU

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Mol	Chain	Res	Type
1	B	43	THR
1	B	61	GLU
1	B	101	ILE
1	C	-327	LEU
1	C	-310	ILE
1	C	-298	GLN
1	C	-287	LYS
1	C	-270	ASN
1	C	-266	ILE
1	C	-187	VAL
1	C	-175	LEU
1	C	-131	LYS
1	C	-112	PHE
1	C	-85	LEU
1	C	-41	ILE
1	C	-35	GLN
1	C	22	LEU
1	C	24	LEU
1	C	43	THR
1	C	61	GLU
1	D	-327	LEU
1	D	-310	ILE
1	D	-298	GLN
1	D	-287	LYS
1	D	-270	ASN
1	D	-266	ILE
1	D	-187	VAL
1	D	-131	LYS
1	D	-112	PHE
1	D	-41	ILE
1	D	-35	GLN
1	D	-8	LYS
1	D	24	LEU
1	D	43	THR
1	D	61	GLU
2	E	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-352	ASN
1	A	-321	GLN

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Mol	Chain	Res	Type
1	A	-152	ASN
1	A	-35	GLN
1	B	-352	ASN
1	B	-169	ASN
1	B	-152	ASN
1	B	-35	GLN
1	C	-352	ASN
1	C	-298	GLN
1	C	-169	ASN
1	C	-152	ASN
1	C	-35	GLN
1	D	-352	ASN
1	D	-298	GLN
1	D	-169	ASN
1	D	-152	ASN
1	D	-35	GLN
1	D	13	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](#)

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](#)

4 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
3	MAL	A	111	-	24,24,24	0.65	0	35,35,35	1.08	1 (2%)
3	MAL	B	111	-	24,24,24	0.57	0	35,35,35	1.18	4 (11%)
3	MAL	C	111	-	24,24,24	0.61	0	35,35,35	0.83	1 (2%)
3	MAL	D	111	-	24,24,24	0.52	0	35,35,35	0.93	1 (2%)

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
3	MAL	A	111	-	-	0/8/48/48	0/2/2/2
3	MAL	B	111	-	-	0/8/48/48	0/2/2/2
3	MAL	C	111	-	-	0/8/48/48	0/2/2/2
3	MAL	D	111	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	111	MAL	O2'-C2'-C3'	-2.06	105.69	110.34
3	B	111	MAL	C1'-O5'-C5'	2.08	117.32	113.47
3	D	111	MAL	C1'-O5'-C5'	2.12	117.39	113.47
3	C	111	MAL	C1'-C2'-C3'	2.46	114.09	110.43
3	A	111	MAL	O5-C5-C4	2.48	114.33	109.68
3	B	111	MAL	C1'-C2'-C3'	2.78	114.56	110.43
3	B	111	MAL	O5'-C1'-C2'	3.71	115.72	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	470/482 (97%)	0.09	4 (0%) 85 86	16, 25, 26, 35	0
1	B	472/482 (97%)	0.19	10 (2%) 67 68	15, 25, 26, 33	0
1	C	462/482 (95%)	0.34	12 (2%) 59 60	9, 25, 26, 31	0
1	D	463/482 (96%)	0.57	53 (11%) 7 5	12, 25, 26, 37	0
2	E	16/17 (94%)	0.87	3 (18%) 2 1	2, 14, 16, 18	0
2	F	16/17 (94%)	0.43	1 (6%) 23 23	9, 16, 27, 27	0
All	All	1899/1962 (96%)	0.30	83 (4%) 38 37	2, 25, 26, 37	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-337	ILE	6.1
1	D	-365	GLY	5.7
1	D	-88	ASN	5.6
1	D	-87	TYR	5.5
1	B	34	GLU	5.3
1	D	-94	ALA	5.1
1	D	-91	PHE	4.8
1	B	102	LEU	4.8
1	D	-95	LEU	4.6
1	D	-343	PHE	4.2
1	D	-368	ILE	3.9
1	D	-363	LEU	3.8
1	D	-92	GLU	3.8
1	D	-339	THR	3.8
1	D	-67	ALA	3.8
1	D	-85	LEU	3.7
1	D	-367	GLU	3.7
1	D	-318	ALA	3.7
1	D	-285	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	-90	LEU	3.7
1	D	-86	LEU	3.6
1	D	-364	LYS	3.6
1	B	67	TYR	3.5
1	D	102	LEU	3.5
1	D	-96	GLU	3.5
1	C	-318	ALA	3.4
1	B	-197	ASN	3.4
1	D	-104	ILE	3.3
1	C	-365	GLY	3.3
1	D	-341	LYS	3.1
1	D	-89	GLU	3.1
2	E	27	ALA	3.1
1	D	-278	PHE	3.1
1	D	-291	ILE	3.1
1	D	-265	ALA	3.1
1	D	-338	GLY	3.1
1	D	-100	SER	3.0
2	E	29	GLU	3.0
1	D	-63	TYR	2.9
1	D	37	TYR	2.9
1	B	70	GLY	2.9
1	D	-264	TYR	2.9
1	D	-289	PRO	2.8
1	A	67	TYR	2.8
1	D	-362	VAL	2.8
1	C	-61	GLU	2.8
1	D	-61	GLU	2.8
1	D	-292	GLU	2.7
1	D	-320	VAL	2.7
1	B	100	PRO	2.7
1	D	-286	ALA	2.7
1	C	37	TYR	2.6
1	C	-102	ALA	2.6
1	D	-279	PRO	2.6
1	D	-366	GLU	2.6
1	D	-336	LYS	2.6
1	D	-66	LEU	2.5
1	B	85	GLU	2.4
1	D	-361	ILE	2.4
2	E	26	ALA	2.4
1	D	-266	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	-346	GLY	2.4
1	A	34	GLU	2.3
1	C	-279	PRO	2.3
1	B	32	ASP	2.3
1	C	-100	SER	2.2
1	D	-283	ASP	2.2
1	D	-280	TYR	2.2
1	B	73	TYR	2.2
1	C	-45	GLN	2.2
1	A	100	PRO	2.2
1	B	-369	LYS	2.2
1	D	26	GLY	2.1
1	D	85	GLU	2.1
1	D	-316	GLY	2.1
2	F	40	ARG	2.1
1	C	-289	PRO	2.1
1	A	59	LEU	2.0
1	C	-291	ILE	2.0
1	D	-65	LYS	2.0
1	D	-198	GLU	2.0
1	C	-278	PHE	2.0
1	C	-296	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAL	A	111	23/23	0.96	0.17	-0.03	26,29,33,36	0
3	MAL	D	111	23/23	0.95	0.18	-0.06	35,44,46,47	0
3	MAL	B	111	23/23	0.95	0.15	-0.56	27,30,33,36	0
3	MAL	C	111	23/23	0.95	0.16	-0.96	38,41,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.