Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:34 pm BST

PDB ID	:	5V51
Title	:	Crystal Structure of MpPR-1i Soaked with Selenourea for 10 min
Authors	:	Luo, Z.; Asojo, O.
Deposited on	:	2017-03-12
Resolution	:	2.92 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
https://www.wwpdb.org/validation/2017/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:

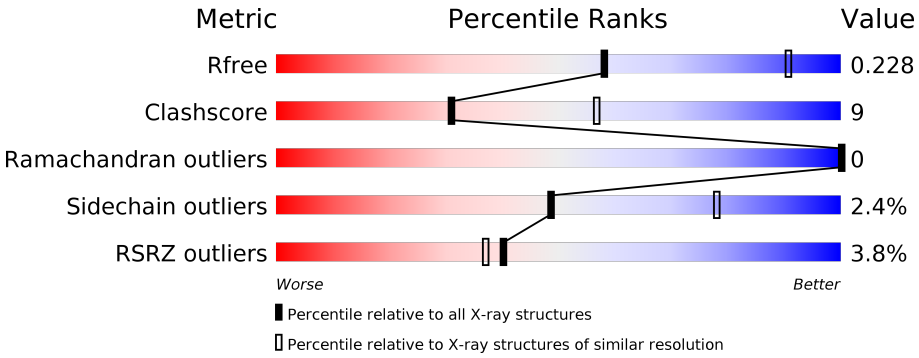
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.92 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 respectively. 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	175	3% 59% 17% 25%
1	B	175	2% 61% 14% 25%
1	C	175	5% 61% 11% 27%
1	D	175	7% 62% 13% 25%
1	E	175	2% 60% 15% 25%
1	F	175	63% 15% 22%

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Mol	Chain	Length	Quality of chain
1	G	175	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7315 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 PR-1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1037	648	178	207	4			
1	B	132	Total	C	N	O	S	0	0	0
			1033	646	177	206	4			
1	C	127	Total	C	N	O	S	0	0	0
			1006	630	172	200	4			
1	D	132	Total	C	N	O	S	0	0	0
			1038	649	178	207	4			
1	E	132	Total	C	N	O	S	0	0	0
			1037	648	178	207	4			
1	F	137	Total	C	N	O	S	0	0	0
			1085	678	187	215	5			
1	G	132	Total	C	N	O	S	0	0	0
			1043	653	178	207	5			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	VAL	-	see remark 999	UNP H6U756
A	167	ARG	-	see remark 999	UNP H6U756
A	168	VAL	-	see remark 999	UNP H6U756
A	169	PRO	-	see remark 999	UNP H6U756
A	170	SER	-	see remark 999	UNP H6U756
A	171	LEU	-	see remark 999	UNP H6U756
A	172	ALA	-	see remark 999	UNP H6U756
A	173	LEU	-	see remark 999	UNP H6U756
A	174	LEU	-	see remark 999	UNP H6U756
A	175	ASN	-	see remark 999	UNP H6U756
A	176	LEU	-	see remark 999	UNP H6U756
A	177	ASP	-	see remark 999	UNP H6U756
A	178	LEU	-	see remark 999	UNP H6U756
A	179	THR	-	see remark 999	UNP H6U756
A	180	THR	-	see remark 999	UNP H6U756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	PRO	-	see remark 999	UNP H6U756
A	182	PHE	-	see remark 999	UNP H6U756
A	183	CYS	-	see remark 999	UNP H6U756
A	184	ASN	-	see remark 999	UNP H6U756
A	185	LEU	-	see remark 999	UNP H6U756
A	186	PRO	-	see remark 999	UNP H6U756
A	187	VAL	-	see remark 999	UNP H6U756
A	188	ASN	-	see remark 999	UNP H6U756
A	189	GLY	-	see remark 999	UNP H6U756
A	190	SER	-	see remark 999	UNP H6U756
A	191	ASN	-	see remark 999	UNP H6U756
A	192	ASP	-	see remark 999	UNP H6U756
A	193	LEU	-	see remark 999	UNP H6U756
A	194	ASP	-	see remark 999	UNP H6U756
A	195	ILE	-	see remark 999	UNP H6U756
A	196	ARG	-	see remark 999	UNP H6U756
A	197	GLU	-	see remark 999	UNP H6U756
B	166	VAL	-	see remark 999	UNP H6U756
B	167	ARG	-	see remark 999	UNP H6U756
B	168	VAL	-	see remark 999	UNP H6U756
B	169	PRO	-	see remark 999	UNP H6U756
B	170	SER	-	see remark 999	UNP H6U756
B	171	LEU	-	see remark 999	UNP H6U756
B	172	ALA	-	see remark 999	UNP H6U756
B	173	LEU	-	see remark 999	UNP H6U756
B	174	LEU	-	see remark 999	UNP H6U756
B	175	ASN	-	see remark 999	UNP H6U756
B	176	LEU	-	see remark 999	UNP H6U756
B	177	ASP	-	see remark 999	UNP H6U756
B	178	LEU	-	see remark 999	UNP H6U756
B	179	THR	-	see remark 999	UNP H6U756
B	180	THR	-	see remark 999	UNP H6U756
B	181	PRO	-	see remark 999	UNP H6U756
B	182	PHE	-	see remark 999	UNP H6U756
B	183	CYS	-	see remark 999	UNP H6U756
B	184	ASN	-	see remark 999	UNP H6U756
B	185	LEU	-	see remark 999	UNP H6U756
B	186	PRO	-	see remark 999	UNP H6U756
B	187	VAL	-	see remark 999	UNP H6U756
B	188	ASN	-	see remark 999	UNP H6U756
B	189	GLY	-	see remark 999	UNP H6U756
B	190	SER	-	see remark 999	UNP H6U756

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	ASN	-	see remark 999	UNP H6U756
B	192	ASP	-	see remark 999	UNP H6U756
B	193	LEU	-	see remark 999	UNP H6U756
B	194	ASP	-	see remark 999	UNP H6U756
B	195	ILE	-	see remark 999	UNP H6U756
B	196	ARG	-	see remark 999	UNP H6U756
B	197	GLU	-	see remark 999	UNP H6U756
C	166	VAL	-	see remark 999	UNP H6U756
C	167	ARG	-	see remark 999	UNP H6U756
C	168	VAL	-	see remark 999	UNP H6U756
C	169	PRO	-	see remark 999	UNP H6U756
C	170	SER	-	see remark 999	UNP H6U756
C	171	LEU	-	see remark 999	UNP H6U756
C	172	ALA	-	see remark 999	UNP H6U756
C	173	LEU	-	see remark 999	UNP H6U756
C	174	LEU	-	see remark 999	UNP H6U756
C	175	ASN	-	see remark 999	UNP H6U756
C	176	LEU	-	see remark 999	UNP H6U756
C	177	ASP	-	see remark 999	UNP H6U756
C	178	LEU	-	see remark 999	UNP H6U756
C	179	THR	-	see remark 999	UNP H6U756
C	180	THR	-	see remark 999	UNP H6U756
C	181	PRO	-	see remark 999	UNP H6U756
C	182	PHE	-	see remark 999	UNP H6U756
C	183	CYS	-	see remark 999	UNP H6U756
C	184	ASN	-	see remark 999	UNP H6U756
C	185	LEU	-	see remark 999	UNP H6U756
C	186	PRO	-	see remark 999	UNP H6U756
C	187	VAL	-	see remark 999	UNP H6U756
C	188	ASN	-	see remark 999	UNP H6U756
C	189	GLY	-	see remark 999	UNP H6U756
C	190	SER	-	see remark 999	UNP H6U756
C	191	ASN	-	see remark 999	UNP H6U756
C	192	ASP	-	see remark 999	UNP H6U756
C	193	LEU	-	see remark 999	UNP H6U756
C	194	ASP	-	see remark 999	UNP H6U756
C	195	ILE	-	see remark 999	UNP H6U756
C	196	ARG	-	see remark 999	UNP H6U756
C	197	GLU	-	see remark 999	UNP H6U756
D	166	VAL	-	see remark 999	UNP H6U756
D	167	ARG	-	see remark 999	UNP H6U756
D	168	VAL	-	see remark 999	UNP H6U756

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Chain	Residue	Modelled	Actual	Comment	Reference
D	169	PRO	-	see remark 999	UNP H6U756
D	170	SER	-	see remark 999	UNP H6U756
D	171	LEU	-	see remark 999	UNP H6U756
D	172	ALA	-	see remark 999	UNP H6U756
D	173	LEU	-	see remark 999	UNP H6U756
D	174	LEU	-	see remark 999	UNP H6U756
D	175	ASN	-	see remark 999	UNP H6U756
D	176	LEU	-	see remark 999	UNP H6U756
D	177	ASP	-	see remark 999	UNP H6U756
D	178	LEU	-	see remark 999	UNP H6U756
D	179	THR	-	see remark 999	UNP H6U756
D	180	THR	-	see remark 999	UNP H6U756
D	181	PRO	-	see remark 999	UNP H6U756
D	182	PHE	-	see remark 999	UNP H6U756
D	183	CYS	-	see remark 999	UNP H6U756
D	184	ASN	-	see remark 999	UNP H6U756
D	185	LEU	-	see remark 999	UNP H6U756
D	186	PRO	-	see remark 999	UNP H6U756
D	187	VAL	-	see remark 999	UNP H6U756
D	188	ASN	-	see remark 999	UNP H6U756
D	189	GLY	-	see remark 999	UNP H6U756
D	190	SER	-	see remark 999	UNP H6U756
D	191	ASN	-	see remark 999	UNP H6U756
D	192	ASP	-	see remark 999	UNP H6U756
D	193	LEU	-	see remark 999	UNP H6U756
D	194	ASP	-	see remark 999	UNP H6U756
D	195	ILE	-	see remark 999	UNP H6U756
D	196	ARG	-	see remark 999	UNP H6U756
D	197	GLU	-	see remark 999	UNP H6U756
E	166	VAL	-	see remark 999	UNP H6U756
E	167	ARG	-	see remark 999	UNP H6U756
E	168	VAL	-	see remark 999	UNP H6U756
E	169	PRO	-	see remark 999	UNP H6U756
E	170	SER	-	see remark 999	UNP H6U756
E	171	LEU	-	see remark 999	UNP H6U756
E	172	ALA	-	see remark 999	UNP H6U756
E	173	LEU	-	see remark 999	UNP H6U756
E	174	LEU	-	see remark 999	UNP H6U756
E	175	ASN	-	see remark 999	UNP H6U756
E	176	LEU	-	see remark 999	UNP H6U756
E	177	ASP	-	see remark 999	UNP H6U756
E	178	LEU	-	see remark 999	UNP H6U756

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Chain	Residue	Modelled	Actual	Comment	Reference
E	179	THR	-	see remark 999	UNP H6U756
E	180	THR	-	see remark 999	UNP H6U756
E	181	PRO	-	see remark 999	UNP H6U756
E	182	PHE	-	see remark 999	UNP H6U756
E	183	CYS	-	see remark 999	UNP H6U756
E	184	ASN	-	see remark 999	UNP H6U756
E	185	LEU	-	see remark 999	UNP H6U756
E	186	PRO	-	see remark 999	UNP H6U756
E	187	VAL	-	see remark 999	UNP H6U756
E	188	ASN	-	see remark 999	UNP H6U756
E	189	GLY	-	see remark 999	UNP H6U756
E	190	SER	-	see remark 999	UNP H6U756
E	191	ASN	-	see remark 999	UNP H6U756
E	192	ASP	-	see remark 999	UNP H6U756
E	193	LEU	-	see remark 999	UNP H6U756
E	194	ASP	-	see remark 999	UNP H6U756
E	195	ILE	-	see remark 999	UNP H6U756
E	196	ARG	-	see remark 999	UNP H6U756
E	197	GLU	-	see remark 999	UNP H6U756
F	166	VAL	-	see remark 999	UNP H6U756
F	167	ARG	-	see remark 999	UNP H6U756
F	168	VAL	-	see remark 999	UNP H6U756
F	169	PRO	-	see remark 999	UNP H6U756
F	170	SER	-	see remark 999	UNP H6U756
F	171	LEU	-	see remark 999	UNP H6U756
F	172	ALA	-	see remark 999	UNP H6U756
F	173	LEU	-	see remark 999	UNP H6U756
F	174	LEU	-	see remark 999	UNP H6U756
F	175	ASN	-	see remark 999	UNP H6U756
F	176	LEU	-	see remark 999	UNP H6U756
F	177	ASP	-	see remark 999	UNP H6U756
F	178	LEU	-	see remark 999	UNP H6U756
F	179	THR	-	see remark 999	UNP H6U756
F	180	THR	-	see remark 999	UNP H6U756
F	181	PRO	-	see remark 999	UNP H6U756
F	182	PHE	-	see remark 999	UNP H6U756
F	183	CYS	-	see remark 999	UNP H6U756
F	184	ASN	-	see remark 999	UNP H6U756
F	185	LEU	-	see remark 999	UNP H6U756
F	186	PRO	-	see remark 999	UNP H6U756
F	187	VAL	-	see remark 999	UNP H6U756
F	188	ASN	-	see remark 999	UNP H6U756

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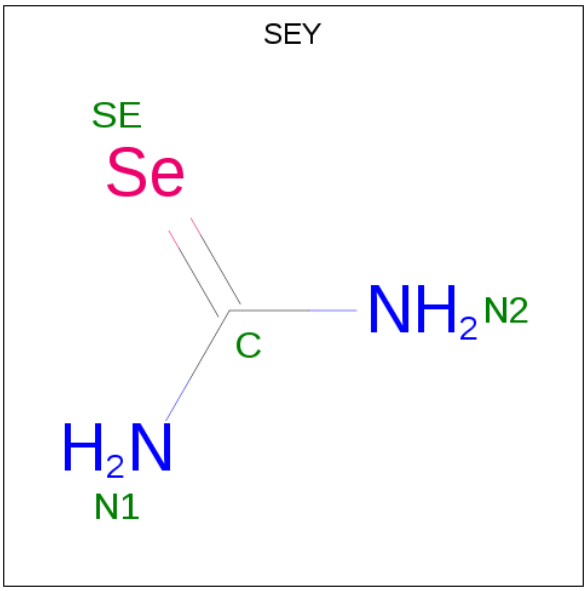
Chain	Residue	Modelled	Actual	Comment	Reference
F	189	GLY	-	see remark 999	UNP H6U756
F	190	SER	-	see remark 999	UNP H6U756
F	191	ASN	-	see remark 999	UNP H6U756
F	192	ASP	-	see remark 999	UNP H6U756
F	193	LEU	-	see remark 999	UNP H6U756
F	194	ASP	-	see remark 999	UNP H6U756
F	195	ILE	-	see remark 999	UNP H6U756
F	196	ARG	-	see remark 999	UNP H6U756
F	197	GLU	-	see remark 999	UNP H6U756
G	166	VAL	-	see remark 999	UNP H6U756
G	167	ARG	-	see remark 999	UNP H6U756
G	168	VAL	-	see remark 999	UNP H6U756
G	169	PRO	-	see remark 999	UNP H6U756
G	170	SER	-	see remark 999	UNP H6U756
G	171	LEU	-	see remark 999	UNP H6U756
G	172	ALA	-	see remark 999	UNP H6U756
G	173	LEU	-	see remark 999	UNP H6U756
G	174	LEU	-	see remark 999	UNP H6U756
G	175	ASN	-	see remark 999	UNP H6U756
G	176	LEU	-	see remark 999	UNP H6U756
G	177	ASP	-	see remark 999	UNP H6U756
G	178	LEU	-	see remark 999	UNP H6U756
G	179	THR	-	see remark 999	UNP H6U756
G	180	THR	-	see remark 999	UNP H6U756
G	181	PRO	-	see remark 999	UNP H6U756
G	182	PHE	-	see remark 999	UNP H6U756
G	183	CYS	-	see remark 999	UNP H6U756
G	184	ASN	-	see remark 999	UNP H6U756
G	185	LEU	-	see remark 999	UNP H6U756
G	186	PRO	-	see remark 999	UNP H6U756
G	187	VAL	-	see remark 999	UNP H6U756
G	188	ASN	-	see remark 999	UNP H6U756
G	189	GLY	-	see remark 999	UNP H6U756
G	190	SER	-	see remark 999	UNP H6U756
G	191	ASN	-	see remark 999	UNP H6U756
G	192	ASP	-	see remark 999	UNP H6U756
G	193	LEU	-	see remark 999	UNP H6U756
G	194	ASP	-	see remark 999	UNP H6U756
G	195	ILE	-	see remark 999	UNP H6U756
G	196	ARG	-	see remark 999	UNP H6U756
G	197	GLU	-	see remark 999	UNP H6U756

- Molecule 2 is selenourea (three-letter code: SEY) (formula: CH_4N_2Se).



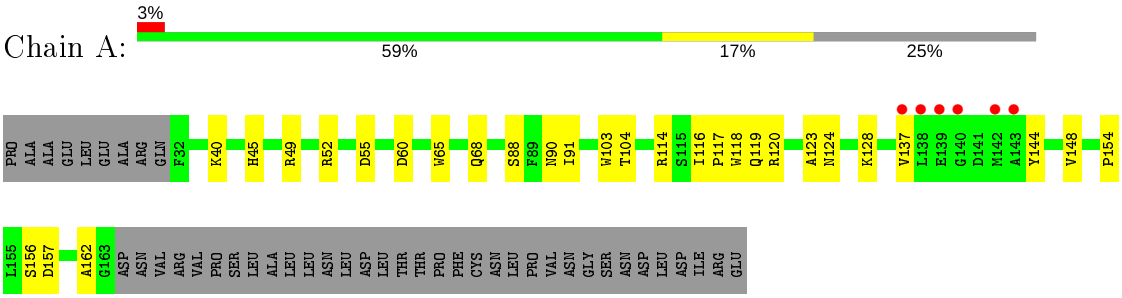
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	Se	0	0
			4	1	2	1		
2	B	1	Total	C	N	Se	0	0
			4	1	2	1		
2	D	1	Total	C	N	Se	0	0
			4	1	2	1		
2	E	1	Total	C	N	Se	0	0
			4	1	2	1		
2	F	1	Total	C	N	Se	0	0
			4	1	2	1		
2	F	1	Total	C	N	Se	0	0
			4	1	2	1		
2	G	1	Total	C	N	Se	0	0
			4	1	2	1		
2	G	1	Total	C	N	Se	0	0
			4	1	2	1		
2	G	1	Total	C	N	Se	0	0
			4	1	2	1		

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 the various outlier classes 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.

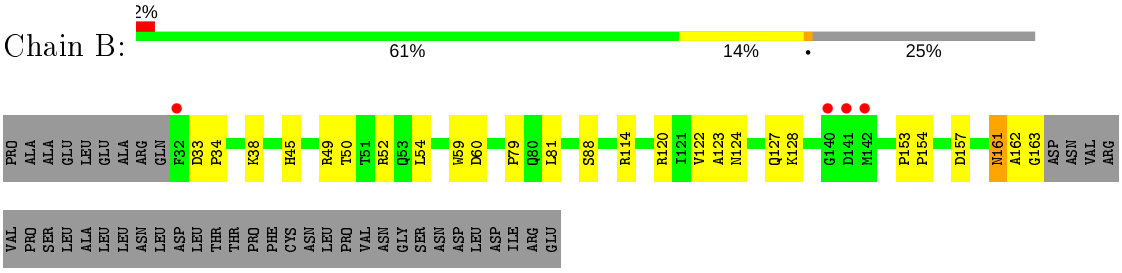
- Molecule 1: PR-1 protein

Chain A:



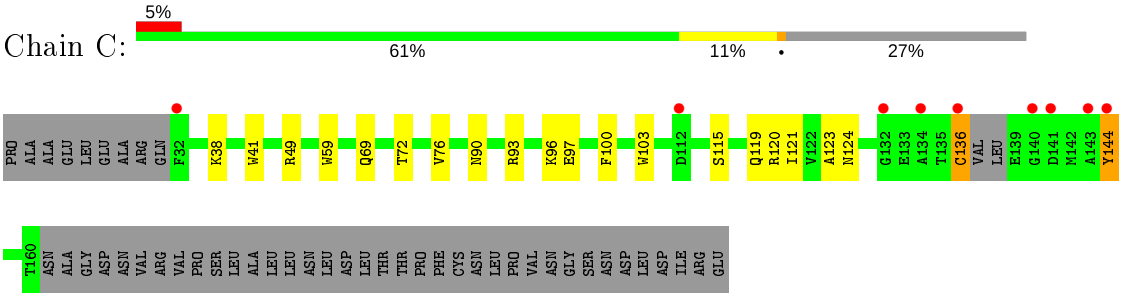
- Molecule 1: PR-1 protein

Chain B:



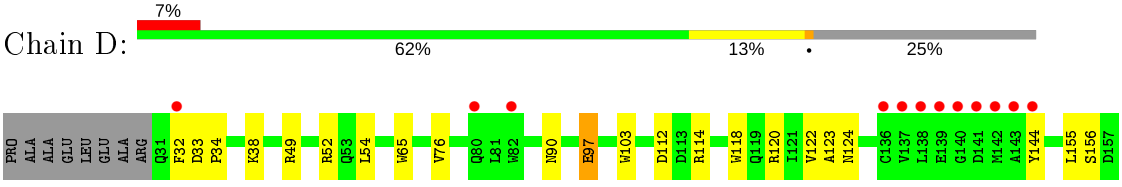
- Molecule 1: PR-1 protein

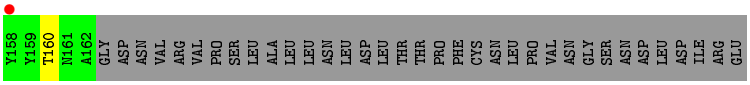
Chain C:



- Molecule 1: PR-1 protein

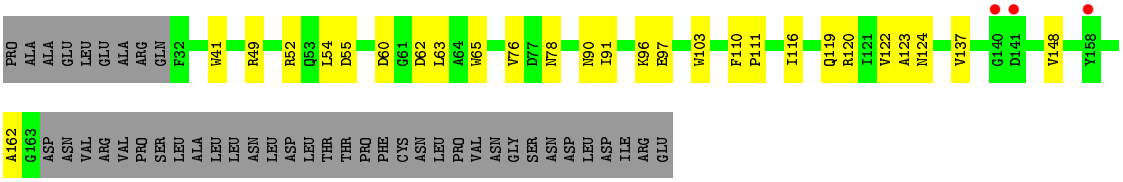
Chain D:





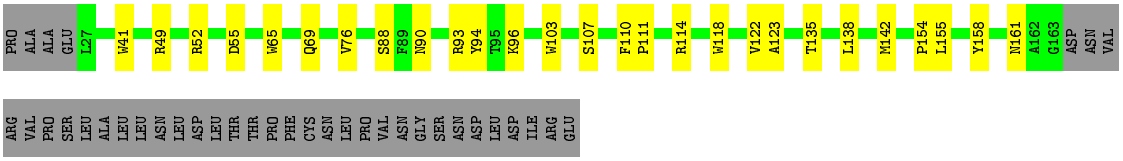
• Molecule 1: PR-1 protein

Chain E:



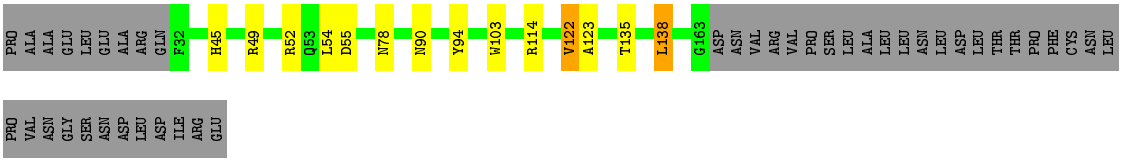
• Molecule 1: PR-1 protein

Chain F:



• Molecule 1: PR-1 protein

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.41Å 81.91Å 130.24Å 90.00° 111.64° 90.00°	Depositor
Resolution (Å)	45.07 – 2.92 45.07 – 2.92	Depositor EDS
% Data completeness (in resolution range)	74.9 (45.07-2.92) 75.0 (45.07-2.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.23 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.187 , 0.228 0.187 , 0.228	Depositor DCC
R_{free} test set	1814 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7315	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	0/1066	0.71	0/1457
1	B	0.52	0/1062	0.72	0/1452
1	C	0.55	0/1034	0.71	0/1411
1	D	0.53	0/1067	0.67	0/1459
1	E	0.54	0/1066	0.70	0/1457
1	F	0.53	0/1114	0.72	0/1520
1	G	0.55	0/1072	0.71	0/1464
All	All	0.54	0/7481	0.71	0/10220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1037	0	928	25	0
1	B	1033	0	922	23	0
1	C	1006	0	897	15	0
1	D	1038	0	927	18	0
1	E	1037	0	928	23	0
1	F	1085	0	987	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1043	0	944	11	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	D	4	0	0	0	0
2	E	4	0	0	1	0
2	F	8	0	0	1	0
2	G	12	0	0	2	0
All	All	7315	0	6533	126	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 9.

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)
1:B:157:ASP:O	1:B:161:ASN:OD1	1.90	0.89
1:D:52:ARG:HG3	1:D:52:ARG:HH11	1.38	0.87
1:A:120:ARG:HG2	1:A:120:ARG:HH11	1.40	0.86
1:D:112:ASP:CG	1:D:114:ARG:HH21	1.82	0.82
1:D:112:ASP:OD1	1:D:114:ARG:NH2	2.14	0.81
1:E:65:TRP:CH2	1:F:52:ARG:HB3	2.18	0.77
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.51	0.76
1:F:76:VAL:HG21	1:F:93:ARG:HH21	1.51	0.74
1:D:120:ARG:HA	1:D:155:LEU:HD11	1.70	0.73
1:A:65:TRP:CH2	1:B:52:ARG:HB3	2.23	0.73
1:A:49:ARG:NH2	1:A:123:ALA:O	2.23	0.71
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.57	0.69
1:D:52:ARG:NH1	1:D:52:ARG:HG3	2.09	0.67
1:D:65:TRP:CH2	1:E:52:ARG:HB3	2.31	0.66
1:C:49:ARG:NH2	1:C:123:ALA:O	2.29	0.65
1:F:88:SER:HB2	1:F:154:PRO:HB3	1.76	0.65
1:E:52:ARG:HG3	1:E:52:ARG:HH11	1.62	0.64
1:E:120:ARG:HG2	1:E:120:ARG:HH11	1.61	0.64
1:C:136:CYS:HB2	1:C:144:TYR:HE1	1.61	0.64
1:B:161:ASN:OD1	1:B:161:ASN:N	2.32	0.63
1:F:135:THR:O	2:F:202:SEY:N2	2.31	0.63
1:A:60:ASP:HB2	1:A:128:LYS:HD2	1.81	0.61
1:F:41:TRP:CZ2	1:F:96:LYS:HG2	2.35	0.61
1:D:97:GLU:H	1:D:97:GLU:CD	2.03	0.61
1:E:65:TRP:HH2	1:F:52:ARG:HB3	1.67	0.58
1:C:38:LYS:HD3	1:C:59:TRP:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.18	0.57
1:B:88:SER:HB2	1:B:154:PRO:HB3	1.87	0.56
1:E:124:ASN:HB2	1:E:162:ALA:HA	1.86	0.56
1:E:97:GLU:OE1	1:E:97:GLU:N	2.24	0.55
1:G:45:HIS:O	1:G:49:ARG:HG3	2.06	0.55
1:B:38:LYS:HD3	1:B:59:TRP:CD2	2.42	0.55
1:D:97:GLU:N	1:D:97:GLU:OE1	2.37	0.54
1:G:94:TYR:HD1	2:G:203:SEY:C	2.20	0.54
1:A:52:ARG:CG	1:A:52:ARG:HH11	2.20	0.54
1:A:45:HIS:O	1:A:49:ARG:HG3	2.08	0.53
1:D:32:PHE:HD2	1:D:34:PRO:HD3	1.73	0.53
1:E:49:ARG:NH1	1:E:55:ASP:O	2.39	0.53
1:F:49:ARG:NH2	1:F:123:ALA:O	2.42	0.52
1:G:49:ARG:NH2	1:G:123:ALA:O	2.43	0.52
1:D:49:ARG:NH2	1:D:123:ALA:O	2.42	0.52
1:E:76:VAL:HA	1:E:91:ILE:HD13	1.90	0.52
1:A:119:GLN:HG2	2:A:201:SEY:SE	2.60	0.52
1:A:65:TRP:HH2	1:B:52:ARG:HB3	1.70	0.52
1:C:100:PHE:CE1	1:C:121:ILE:HD13	2.45	0.51
1:E:78:ASN:O	1:E:78:ASN:ND2	2.39	0.51
1:B:60:ASP:HB2	1:B:128:LYS:HD3	1.93	0.51
1:E:49:ARG:NH2	1:E:123:ALA:O	2.44	0.51
1:G:135:THR:H	2:G:202:SEY:SE	2.44	0.50
1:F:52:ARG:HH11	1:F:52:ARG:HG3	1.77	0.50
1:D:38:LYS:HD2	1:E:111:PRO:HD2	1.93	0.50
1:B:124:ASN:ND2	1:B:163:GLY:H	2.09	0.49
1:E:60:ASP:HB3	1:E:63:LEU:HD12	1.93	0.49
1:C:115:SER:O	1:C:119:GLN:HG3	2.12	0.49
1:D:156:SER:HB3	1:D:160:THR:HG21	1.94	0.49
1:B:124:ASN:HD22	1:B:163:GLY:H	1.61	0.49
1:C:90:ASN:HB3	1:C:103:TRP:CE2	2.48	0.49
1:D:90:ASN:HB3	1:D:103:TRP:CZ2	2.48	0.49
1:E:41:TRP:CZ2	1:E:96:LYS:HG2	2.48	0.49
1:D:90:ASN:HB3	1:D:103:TRP:CE2	2.48	0.48
1:C:76:VAL:HG21	1:C:93:ARG:HH22	1.77	0.48
1:A:137:VAL:HG23	1:A:137:VAL:O	2.13	0.48
1:D:54:LEU:CD2	1:D:124:ASN:OD1	2.61	0.48
1:E:120:ARG:NH1	1:E:120:ARG:HG2	2.27	0.48
1:E:52:ARG:HG3	1:E:52:ARG:NH1	2.28	0.48
1:G:49:ARG:NH1	1:G:55:ASP:O	2.47	0.48
1:A:120:ARG:CG	1:A:120:ARG:HH11	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HB3	1:B:54:LEU:HB2	1.96	0.48
1:A:124:ASN:HB2	1:A:162:ALA:HA	1.96	0.48
1:E:90:ASN:HB3	1:E:103:TRP:CE2	2.49	0.47
1:G:49:ARG:HB3	1:G:54:LEU:HB2	1.95	0.47
1:A:116:ILE:N	1:A:117:PRO:HD2	2.29	0.47
1:C:38:LYS:HD3	1:C:59:TRP:CE2	2.49	0.47
1:C:120:ARG:HH11	1:C:120:ARG:CG	2.27	0.47
1:G:78:ASN:O	1:G:78:ASN:ND2	2.47	0.47
1:A:49:ARG:NH1	1:A:55:ASP:O	2.48	0.46
1:G:90:ASN:HB3	1:G:103:TRP:CE2	2.50	0.46
1:B:161:ASN:HB2	2:B:201:SEY:C	2.45	0.46
1:A:88:SER:HB2	1:A:154:PRO:HB3	1.97	0.46
1:C:41:TRP:CE2	1:C:96:LYS:HG2	2.51	0.46
1:A:40:LYS:HA	1:A:40:LYS:HD2	1.73	0.46
1:E:137:VAL:O	1:E:137:VAL:HG23	2.15	0.45
1:B:49:ARG:NH2	1:B:123:ALA:O	2.50	0.45
1:F:118:TRP:O	1:F:122:VAL:HG22	2.17	0.45
1:E:110:PHE:CD2	1:E:110:PHE:C	2.90	0.45
1:A:144:TYR:CD1	1:A:144:TYR:O	2.70	0.44
1:B:79:PRO:HG2	1:B:81:LEU:HD21	2.00	0.44
1:E:123:ALA:HA	2:E:201:SEY:N2	2.33	0.44
1:B:120:ARG:HH11	1:B:120:ARG:HG2	1.82	0.44
1:E:91:ILE:HG13	1:E:148:VAL:HG22	1.99	0.44
1:A:90:ASN:HB3	1:A:103:TRP:CE2	2.52	0.44
1:F:93:ARG:HG3	1:F:94:TYR:CE2	2.53	0.44
1:F:49:ARG:NH1	1:F:55:ASP:O	2.48	0.43
1:A:104:THR:HA	1:A:118:TRP:HD1	1.83	0.43
1:B:38:LYS:HD3	1:B:59:TRP:CE2	2.53	0.43
1:E:116:ILE:HA	1:E:119:GLN:HG3	2.01	0.43
1:A:156:SER:HB3	1:A:157:ASP:H	1.56	0.43
1:D:118:TRP:O	1:D:122:VAL:HG22	2.18	0.43
1:F:107:SER:HB3	1:F:118:TRP:CD2	2.53	0.43
1:G:138:LEU:HD23	1:G:138:LEU:HA	1.62	0.43
1:D:144:TYR:CD1	1:D:144:TYR:N	2.87	0.43
1:A:120:ARG:CG	1:A:120:ARG:NH1	2.77	0.42
1:D:33:ASP:HA	1:D:34:PRO:HD2	1.68	0.42
1:C:97:GLU:OE1	1:C:97:GLU:N	2.42	0.42
1:C:69:GLN:O	1:C:72:THR:HG22	2.20	0.42
1:F:110:PHE:CD1	1:F:111:PRO:HA	2.55	0.42
1:B:127:GLN:HG2	1:B:153:PRO:HD3	2.00	0.42
1:B:114:ARG:HG3	1:B:114:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:VAL:HG21	1:F:93:ARG:NH2	2.28	0.42
1:B:124:ASN:HB3	1:B:162:ALA:HA	2.02	0.42
1:G:122:VAL:HG13	1:G:122:VAL:O	2.19	0.42
1:B:33:ASP:HA	1:B:34:PRO:HD2	1.88	0.41
1:C:144:TYR:O	1:C:144:TYR:CD1	2.73	0.41
1:F:155:LEU:HD22	1:F:161:ASN:ND2	2.36	0.41
1:F:158:TYR:CD1	1:F:158:TYR:C	2.94	0.41
1:F:65:TRP:CH2	1:G:52:ARG:HB3	2.55	0.41
1:F:90:ASN:HB3	1:F:103:TRP:CE2	2.56	0.41
1:A:91:ILE:HG13	1:A:148:VAL:HG22	2.02	0.41
1:B:45:HIS:O	1:B:49:ARG:HG3	2.20	0.41
1:B:38:LYS:HD3	1:B:59:TRP:CG	2.56	0.41
1:A:68:GLN:HG2	1:A:68:GLN:O	2.21	0.40
1:C:120:ARG:NH1	1:C:120:ARG:CG	2.83	0.40
1:A:52:ARG:NH1	1:A:52:ARG:CG	2.80	0.40
1:B:124:ASN:CB	1:B:162:ALA:HA	2.51	0.40
1:B:38:LYS:HB2	1:B:38:LYS:HE2	1.92	0.40
1:E:54:LEU:HA	1:E:54:LEU:HD23	1.86	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	130/175 (74%)	125 (96%)	5 (4%)	0	100	100
1	B	130/175 (74%)	126 (97%)	4 (3%)	0	100	100
1	C	123/175 (70%)	118 (96%)	5 (4%)	0	100	100
1	D	130/175 (74%)	120 (92%)	10 (8%)	0	100	100
1	E	130/175 (74%)	123 (95%)	7 (5%)	0	100	100
1	F	135/175 (77%)	128 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	130/175 (74%)	123 (95%)	7 (5%)	0	100 100
All	All	908/1225 (74%)	863 (95%)	45 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	107/149 (72%)	106 (99%)	1 (1%)	78 92
1	B	106/149 (71%)	103 (97%)	3 (3%)	43 75
1	C	104/149 (70%)	101 (97%)	3 (3%)	42 74
1	D	107/149 (72%)	105 (98%)	2 (2%)	57 83
1	E	107/149 (72%)	105 (98%)	2 (2%)	57 83
1	F	113/149 (76%)	109 (96%)	4 (4%)	36 68
1	G	109/149 (73%)	106 (97%)	3 (3%)	43 75
All	All	753/1043 (72%)	735 (98%)	18 (2%)	49 78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	B	50	THR
1	B	122	VAL
1	B	161	ASN
1	C	124	ASN
1	C	136	CYS
1	C	144	TYR
1	D	76	VAL
1	D	97	GLU
1	E	62	ASP
1	E	122	VAL
1	F	69	GLN

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Mol	Chain	Res	Type
1	F	114	ARG
1	F	138	LEU
1	F	142	MET
1	G	114	ARG
1	G	122	VAL
1	G	138	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	ASN
1	C	98	GLN
1	E	98	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

9 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	SEY	D	201	-	3,3,3	0.37	0	3,3,3	0.25	0
2	SEY	F	201	-	3,3,3	0.26	0	3,3,3	0.32	0
2	SEY	E	201	-	3,3,3	0.33	0	3,3,3	0.28	0
2	SEY	G	201	-	3,3,3	0.33	0	3,3,3	0.25	0
2	SEY	B	201	-	3,3,3	0.33	0	3,3,3	0.26	0
2	SEY	A	201	-	3,3,3	0.35	0	3,3,3	0.27	0
2	SEY	G	202	-	3,3,3	0.62	0	3,3,3	0.20	0
2	SEY	G	203	-	3,3,3	0.67	0	3,3,3	0.18	0
2	SEY	F	202	-	3,3,3	0.46	0	3,3,3	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	SEY	1	0
2	B	201	SEY	1	0
2	A	201	SEY	1	0
2	G	202	SEY	1	0
2	G	203	SEY	1	0
2	F	202	SEY	1	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	132/175 (75%)	0.30	6 (4%) 33 30	37, 68, 128, 179	0
1	B	132/175 (75%)	0.21	4 (3%) 50 46	36, 70, 116, 175	0
1	C	127/175 (72%)	0.44	9 (7%) 16 13	49, 82, 126, 148	0
1	D	132/175 (75%)	0.54	13 (9%) 7 6	48, 84, 122, 149	0
1	E	132/175 (75%)	0.14	3 (2%) 60 59	40, 67, 106, 161	0
1	F	137/175 (78%)	0.12	0 100 100	31, 53, 101, 136	0
1	G	132/175 (75%)	0.02	0 100 100	31, 58, 97, 115	0
All	All	924/1225 (75%)	0.25	35 (3%) 40 37	31, 70, 119, 179	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	4.3
1	A	140	GLY	4.2
1	D	138	LEU	3.9
1	D	140	GLY	3.8
1	B	141	ASP	3.7
1	B	32	PHE	3.2
1	E	141	ASP	3.2
1	C	141	ASP	3.2
1	C	112	ASP	3.1
1	C	32	PHE	3.1
1	C	132	GLY	3.0
1	D	141	ASP	3.0
1	A	139	GLU	3.0
1	A	137	VAL	2.9
1	A	143	ALA	2.9
1	C	144	TYR	2.9
1	A	138	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	139	GLU	2.8
1	C	134	ALA	2.7
1	D	143	ALA	2.7
1	D	142	MET	2.7
1	D	82	TRP	2.5
1	D	32	PHE	2.5
1	D	158	TYR	2.5
1	D	144	TYR	2.3
1	A	142	MET	2.3
1	B	142	MET	2.3
1	E	140	GLY	2.3
1	D	136	CYS	2.3
1	D	80	GLN	2.2
1	C	143	ALA	2.2
1	C	140	GLY	2.1
1	D	137	VAL	2.1
1	E	158	TYR	2.0
1	C	136	CYS	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. 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	B-factors(Å^2)	Q<0.9
2	SEY	G	202	4/4	0.89	0.25	63,82,84,102	4
2	SEY	G	203	4/4	0.92	0.28	50,58,59,73	4
2	SEY	F	202	4/4	0.94	0.18	76,77,84,93	4
2	SEY	D	201	4/4	0.95	0.17	51,56,69,88	4
2	SEY	E	201	4/4	0.98	0.27	59,74,74,75	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SEY	G	201	4/4	0.98	0.17	43,56,59,67	4
2	SEY	B	201	4/4	0.98	0.30	96,102,116,135	4
2	SEY	A	201	4/4	0.99	0.19	33,47,60,62	4
2	SEY	F	201	4/4	0.99	0.20	38,50,51,62	4

6.5 Other polymers (i)

There are no such residues in this entry.